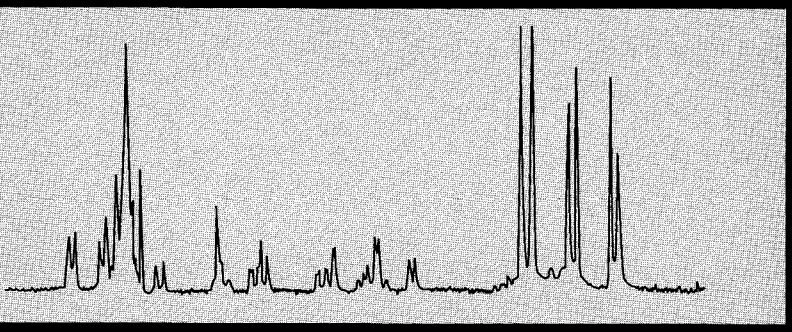
Chemical Information

1992



NCI Investigational Drugs

U.S. DEPARTMENT OF HEALTH
AND HUMAN SERVICES
Public Health Services
National Institutes of Health

NIH Publication No. 92-2654
March 1992

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COVER

On the cover is a photograph of crystals of Taxol. Also depicted is the proton NMR spectrum of this molecule.

This Edition of the

NCI Investigational Drugs - Chemical Information

is Dedicated to the Memory of

Dr. Robert C. Moore

PREFACE

NCI Investigational Drugs - Chemical Information has been prepared by the Pharmaceutical Resources Branch, Developmental Therapeutics Program, Division of Cancer Treatment, National Cancer Institute. The chemical information presented was obtained from National Cancer Institute contractors. The following organizations and individuals contributed to the preparation of this book:

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INTRODUCTION

NCI Investigational Drugs - Chemical Information is designed to provide selected relevant chemical and physical data to investigators involved in various multidisciplinary studies of drugs which were developed or are being developed by the Developmental Therapeutics Program, Division of Cancer Treatment, National Cancer Institute. Monographs are presented on most of the investigational agents currently distributed by the Division of Cancer Treatment for clinical study. Monographs are also presented for many compounds in preclinical development.

Selected chemical information is presented in a standardized format to facilitate the retrieval of specific information. The format includes the chemical name, common names, molecular formula, molecular weight and structure of each compound. Generally, approximate solubility, stability, ultraviolet absorption, and chromatographic information are provided. Occasionally other selected data are provided (e.g., optical rotation).

The approximate solubility data are generated during the early stages of drug development. These studies are not necessarily conducted under "saturation conditions" and are intended only to provide rough solubility estimates for guidance during the formulation development process. As such, they should be useful for providing leads such as the potential suitability of a particular solvent as a vehicle for animal studies or for use in extracting the drug from biological fluids.

The bulk drug stability data provided are also generated early in the development process. These studies are intended to identify potential stability problems as well as identify a possible storage condition for the bulk drug. The data are not intended to support long term stability during storage. They can, however, be used as a general guide as to the relative stability of the bulk drug. The

solution stability data may provide guidance as to the storage of solutions prepared from bulk drug (e.g., some solutions may need to be prepared immediately before use).

Data from some analytical testing are presented as a range of values. These ranges are derived from the assay of multiple bulk drug samples and are typical of the values that were generated from the better samples received for analysis. Unless otherwise indicated, samples are assayed on an "as is" basis. Corrections for water content are not generally applied.

The chromatographic procedures provided [usually high performance liquid chromatographic (HPLC) procedures] are those which were developed by the analytical contractors and have been used for the assay of multiple lots of bulk drugs and clinical drug products. As such, the methods may not be immediately useful for other applications. For example, the inclusion of an extraction/isolation step or a change in detection mode may be necessary to allow the quantitation of drug in biological fluids. However, the methods can provide a starting point for developing these more specialized procedures, thus eliminating some of the time spent on methods development. It should be noted that the HPLC columns listed in the method description are the actual columns used in our analyses of the material. This is not to imply that other similar columns will not perform as well or, perhaps, better. Also, it should be recognized that the transfer of HPLC methodology from laboratory to laboratory is likely to require some amount of "fine tuning" and that retention volumes and other chromatographic characteristics may not be identical for a given set of operating conditions.

Toxicity data were derived from the Registry of Toxic Effects of Chemical Substances compiled by the National Institute of Occupational Safety and Health, the Toxicology Branch (NCI) and *in vivo* screening data (NCI). These data are provided for general

guidance only and no warranty of accuracy is implied by their inclusion. Further information should be obtained from the primary source.

Additional analytical chemistry information is available upon request from the Pharmaceutical Resources Branch, National Cancer Institute.

For information on the pharmaceutical dosage forms refer to the companion publication **NCI Investigational Drugs: Pharmaceutical Data.**

Copies of these publications or questions pertaining to the drugs contained therein may be addressed to:

Chief, Pharmaceutical Resources Branch
Developmental Therapeutics Program
National Cancer Institute
Executive Plaza North, Room 818
Bethesda, Maryland 20892
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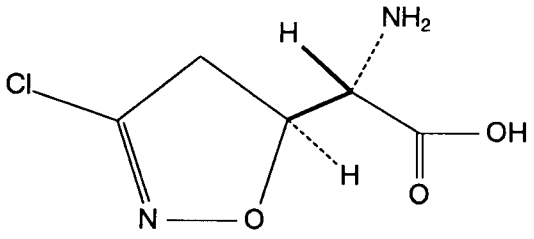
ACIVICIN

NSC - 163501



Chemical Name:
α-Amino-3-chloro-4,5-dihydro-5-isoxazoleacetic acid, [*S*-(*R**,*R**)]-

Other Names: AT-125; U-42126

CAS Registry #: 42228-92-2

Molecular Formula: $C_5H_7ClN_2O_3$ **M.W. :** 178.6

Approximate Solubility:	(mg/mL)
Water	17.9 - 18.2
0.1 M Citrate buffer pH 4.3	17.1 - 25.7
0.1 M Borate buffer pH 9.0	8.7 - 13.0
0.1 N HCl	31 - 35
0.1 N NaOH	34.4 - 36.8
95% Ethanol	0.8
10% Ethanol	8.2 - 16.4

Methanol	0.8
Chloroform	0.9

Stability:

Bulk:
A sample stored at 60 °C for 14 days showed no decomposition as indicated by UV absorption, paper chromatography, or ionic chloride determination.

Solution:
An aqueous solution (18 mg/mL) which was stored at 28 °C for 14 days showed less than 1% decomposition by UV absorption, paper chromatography and ionic chloride measurement.

Ultraviolet Absorption:

(H_2O)

λ_{max} = 218 ± 2 nm ε = 3,500 - 3,700

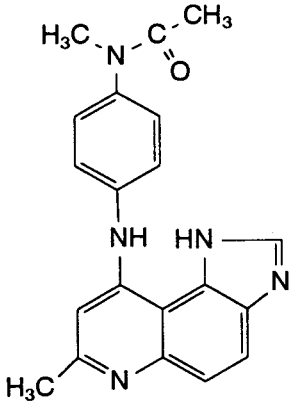
High Performance Liquid Chromatography:

Column:	μ-Bondapak C_{18} 300 x 3.9 mm i.d. (Waters Associates)
Mobile Phase:	Water containing 0.0075 M heptanesulfonic acid, pH 2.5
Flow Rate:	1.0 mL/min

Detection:	UV at 218 nm
Sample Preparation:	1.0 mg/mL in water or internal standard solution
Internal Standard:	Nicotinic acid (0.825 mg/mL in water)
Retention Volume:	5.4 mL (NSC-163501) 7.8 mL (I.S.)

ACODAZOLE HYDROCHLORIDE

NSC - 305884



* HCl

Chemical Name:
N-Methyl-*N*-[4-[(7-methyl-1*H*-imidazo(4,5-*f*)quinolin-9-yl)amino]phenyl]acetamide, monohydrochloride

CAS Registry Number: 55435-65-9

Molecular Formula: $C_{20}H_{19}N_5O \cdot HCl$ **M.W. :** 381.9

Approximate Solubility:	(mg/mL)
H_2O	> 50
pH 4 Acetate buffer	> 50

pH 9 Carbonate buffer	> 50
10% Ethanol	> 50
Methanol	10 - 12
95% Ethanol	10 - 15
0.1 N HCl	> 50
0.1 N NaOH	< 1

Stability:

Bulk:

The bulk compound did not undergo significant decomposition when heated at 60 °C for 30 days in the dark (HPLC). The compound is quite hygroscopic.

Solution:

A solution (0.1 mg/mL) prepared in unbuffered water and stored at room temperature and exposed to light was stable for > 48 hours (HPLC).

Ultraviolet Absorption:

(Methanol)

λ_{max}	ε
345 ± 2 nm	15,300 - 16,600
316 ± 2 nm	12,400 - 13,200
255 ± 2 nm	27,900 - 30,500
227 ± 2 nm	21,100 - 22,400

High Performance Liquid Chromatography:

Column:	μ-Bondapak C_{18}, 300 x 3.9 mm ID (Waters Assoc.)
Mobile Phase:	Methanol/water (containing 2% acetic acid), 40/60 (v/v)
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Internal Standard:	Acetophenone, 1.28 μg/mL
Retention Volume:	25.0 mL (NSC-305884) 13.0 mL (I.S.)

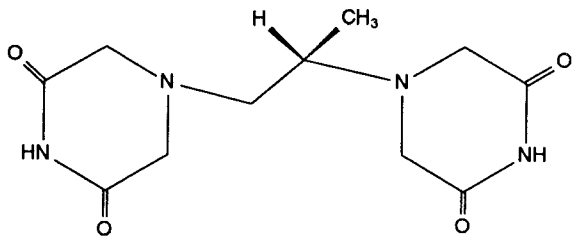
Toxicity Data:

Mouse(ip): LD_{50}: 161 mg/kg
NCI Screening Program Data Summary

Mouse(iv): LD_{50}: 87,590 μg/kg
NCI Screening Program Data Summary

ADR-529

NSC - 169780



Chemical Name:
4,4′-(1-Methyl-1,2-ethanediyl)bis-2,6-piperazinedione,(+)-

Other Names:
Dexrazoxane (USAN/INN); ICRF-187

CAS Registry Number: 24584-09-6

Molecular Formula: $C_{11}H_{16}N_4O_4$ **M.W.:** 268.3

Approximate Solubility:	(mg/mL)
H_20	10 - 12
0.1 N HCl	35 - 43
0.1 N NaOH	25 - 34
10% EtOH	6.7 - 10
MeOH	1
H_2O/DMA(1:1)	7.1 - 10
0.1 M Citrate Buffer (pH 4)	9.7 -14.5
0.1 M Borate Buffer (pH 9)	8.7 - 13

Stability:

Bulk:
A sample stored at 60 °C showed less than 1% decomposition after seven days (HPLC).

Solution:
A 10 mg/mL solution in water at 28 °C showed 10% and 42% decomposition in 1 day and 6 days respectively (HPLC).

High Performance Liquid Chromatography:

Column:	μBondapak C_{18} 300 x 3.9 mm i.d.
Mobile Phase:	CH_3CN/pH 7 0.01 M phosphate buffer, 10/90, v/v
Flow Rate:	1 mL/min
Detection:	UV at 200 nm
Sample Preparation:	0.05 mg/mL in internal standard solution
Internal Standard:	Acetanilide (0.08 mg/mL in CH_3CN/0.01 M phosphate buffer, pH 7,3.5/96.5, v/v)
Retention Volume:	6.6 mL (NSC-169780) 19.5 mL (I.S.)

Optical Rotation:

(c = 0.5, H_2O) $[\alpha]_D^{20} = +42 \pm 2°$

Toxicity Data:

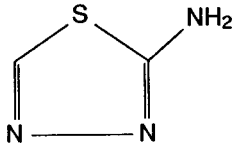
Man(iv): TD_{Lo}: 383 mg/kg
Cancer Clinical Trials, 4,143,(1981)

Mouse(ip): LD_{Lo}: 800 mg/kg
Drugs of the Future,2,473,(1977)

Dog(iv): LD_{Lo}: 2 gm/kg
Cancer Treatment Reports,64,1211,(1980)

AMINOTHIADIAZOLE

NSC - 4728



Chemical Name: 1,3,4-Thiadiazol-2-amine

CAS Registry Number: 4005-51-0

Molecular Formula: $C_2H_3N_3S$ **M.W.:** 101.1

Approximate Solubility: (mg/mL)

0.1 N HCL	22
4.0 N HCL	400
Water	20
Ethanol	17
Chloroform	0.35
Benzene	< 0.05
Ethyl acetate	0.8

Stability:

Bulk:
A sample stored for four weeks at 60 °C showed no

decomposition (UV,TLC).

Solution:
A solution (10 mg/mL) showed no decomposition after twenty-four hours at room temperature (UV,TLC).

Ultraviolet Absorption:

(H_2O)

λ_{max} = 250 ± 2 nm ε = 4,120 - 4,520

High Performance Liquid Chromatography:

Column:	50 cm x 4 mm i.d. Zorbax C-8
Mobile Phase:	0.1% Diethylamine in pH 6.5, 0.05 M KH_2PO_4/methanol (99/1)
Flow Rate:	2 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.5 mg/mL in 0.1 N HCL or internal standard solution
Internal Standard:	Guanosine (1 mg/mL in 0.1 N HCL)
Retention Volume:	8.0 mL (NSC - 4728) 12.5 mL (I.S.)

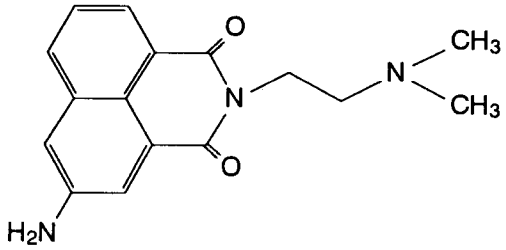
Toxicity Data:

Rat(ip): LD_{50}: 200 mg/kg
Takeda Kenkyusho Ho, 35,68,(1976)

Rat(sc): LD_{50}: 200 mg/kg
Johns Hopkins Medical Journal, 130,95 (1972)

AMONAFIDE

NSC - 308847



Chemical Name:
5-Amino-2-[2-(dimethylamino)ethyl]-1*H*-benz[*de*]isoquinoline-1,3(2*H*)-dione

Other Names:
Nafidimide; Amonafide HCl (NSC-621093)

CAS Registry Number: 69408-81-7

Molecular Formula: $C_{16}H_{17}N_3O_2$ **M.W.:** 283.3

Approximate Solubility:	(mg/mL)
H_2O	< 1
pH 4 acetate buffer	≈10
pH 9 carbonate buffer	< 1
0.1 N HCl	≈20
0.1 N NaOH	< 1
10% Ethanol	< 1
95% Ethanol	5 - 7
95% Methanol	5 - 7

Stability:

Bulk:
A sample stored at 60 °C for 30 days assayed at > 99% (HPLC).

Solution:
A 0.4 mg/mL solution of drug in 0.2 M acetate buffer (pH4.0) showed no decomposition after 48 hours at room temperature (HPLC).

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 300 x 3.9 mm i.d.
Mobile Phase:	CH_3CN/0.005 M heptanesulfonic acid adjusted to pH 2.5 with H_2SO_4, 32/68, v/v.
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.04 mg/mL in CH_3CN/0.005 M heptanesulfonic acid adjusted to pH 2.5 with H_2SO_4 (5/75,v/v) containing internal standard.
Internal Standard:	Indole, 0.2 mg/mL
Retention Volume:	8.3 mL (NSC-308847) 20.1 mL (I.S.)

Ultraviolet Absorption:

(MeOH)

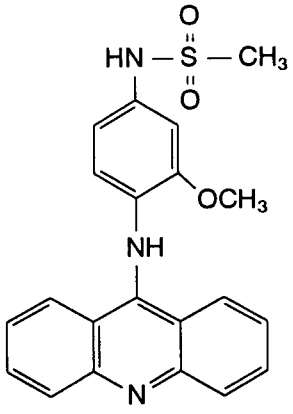
λ_{max}	ε
217 ± 2nm	27,200 - 29,400
249 ± 2nm	26,000 - 27,200
342 ± 2nm	8,050 - 8,450
422 ± 2nm	4,200 - 4,400

Toxicity Data:

Mouse(iv): LD_{50}: 69 mg/kg
National Technical Information Service, PB84-219542

AMSACRINE

NSC - 249992



Chemical Name:
N-[4-(9-Acridinylamino)-3-methoxyphenyl]methanesulfonamide

Other Names:
m-AMSA; Acridinyl anisidide

CAS Registry Number: 51264-14-3

Molecular Formula: $C_{21}H_{19}N_3O_3S$ **M.W.:** 393.5

Approximate Solubility:	(mg/mL)
Water	< 1.0
pH 4 buffer	< 1.0
pH 9 buffer	< 1.0
10% EtOH	< 1.0
95% EtOH	1.5 - 1.8
MeOH	2.9 - 3.2
$CHCl_3$	1.0

Stability:

Bulk:
A sample stored at 60 °C for 30 days showed no decomposition (IR, TLC or UV).

Solution:
A sample was dissolved in methanol and diluted with water (1:33). No decomposition was detected by UV after standing 4 days at room temperature and exposed to light.

Ultraviolet Absorption:

(pH 4 acetate buffer)

λ_{max}	ε
265 ± 2 nm	48,400 - 49,000
430 ± 2 nm	13,050 - 13,250

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 300 x 4 mm i.d.
Mobile Phase:	CH_3CN/5 μM heptanesulfonic acid, pH 2.8, (35/65,v/v)
Flow Rate:	1 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.4 mg/mL in acetonitrile containing internal standard

Internal Standard:	Butyrophenone, 1.3 μL/mL in acetonitrile
Retention Volume:	8.25 mL (NSC-249992) 13.5 mL (I.S)

Toxicity Data:

Human(iv): TD_{Lo}: 12 mg/kg
Cancer Research, 38,3712,(1978)

Mouse(po): LD_{50}: 53420 μg/kg
NCI Screening Program Data Summary

Mouse(ip): LD_{50}: 15470 μg/kg
NCI Screening Program Data Summary

Mouse(sc): LD_{50}: 110 mg/kg
NCI Screening Program Data Summary

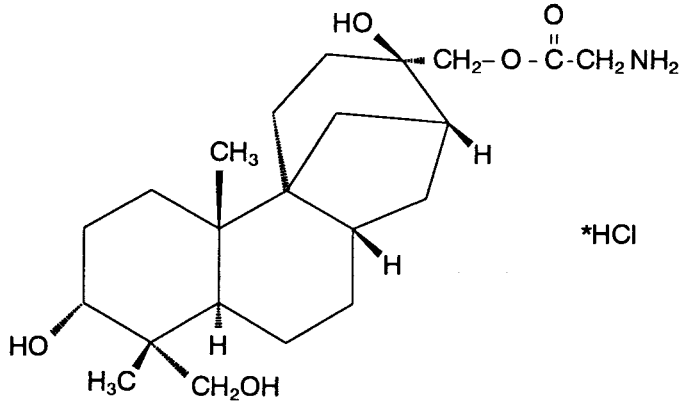
Mouse(iv): LD_{50}: 33700 μg/kg
Cancer Treatment Reports, 64,855,(1980)

Dog(po): LD_{50}: 50 mg/kg
Cancer Treatment Reports, 66,1939,(1982)

Dog(iv): LD_{50}: 6250 μg/kg
Cancer Treatment Reports, 64,855,(1980)

APHIDICOLIN GLYCINATE

NSC - 303812



Chemical Name:
Glycine, (tetradecahydro-3,9-dihydroxy-4-(hydroxymethyl)-4,11b-dimethyl-8,11a-methano-11a*H*-cyclohepta(*a*)naphthalen-9-yl)methyl ester, hydrochloride, (3*R*-(3α,4α,4aα,6aβ,8β,9β,11aβ,11bβ)-

Other Names:
Aphidicolin-17-glycinate; ICI 137233

CAS Registry Number: 92803-82-2

Molecular Formula: $C_{22}H_{37}NO_5 \cdot HCl$ **M.W.:** 432.0

Approximate Solubility:	(mg/mL)
H_2O	100
MeOH	100
$CHCl_3$	< 0.001

Stability:

Bulk:
Compound is stable at 25 ± 2 °C under normal illumination or in the dark and at 45 °C for at least 4 weeks (HPLC).

Solution:
An 8 mg/mL solution in water at room temperature (25 ± 2°C) decomposes at an apparent linear rate of 0.20 ± 0.05% per hour over a 24 hour period.

Ultraviolet Absorption:
Exhibits end absorption only.

High Performance Liquid Chromatography:

Column:	Versapack C_{18}, 10 μm, x 4.6 mm i.d.
Mobile Phase:	35% acetonitrile/water, containing 0.01M sodium decylsulfate (adjusted to pH 3.0 with sulfuric acid)
Flow Rate:	2 mL/min
Detection:	Model 410 Differential Refractometer (Waters Assoc.). Range=64, positive polarity
Sample Preparation:	≈2.5 mg/mL in mobile phase

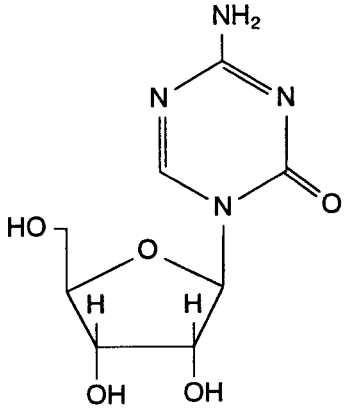
Internal Standard:	Valerophenone, ≈2.5 mg/mL in mobile phase
Retention Volume:	14.0 mL (NSC 303812) 23.8 mL (I.S.)

Optical Rotation:

(c = 1, MeOH) $[\alpha]_D^{20} = +4.5 \pm 0.5°$

AZACITIDINE

NSC - 102816



Chemical Name:
4-Amino-1-β-*D*-ribofuranosyl-1,3,5-triazin-1(1*H*)-one

Other Names:
Azacitidine (USAN); 5-Azacytidine; Ladakamycin

CAS Registry Number: 320-67-2

Molecular Formula: $C_8H_{12}N_4O_5$ **M.W.:** 244.2

Approximate Solubility:	(mg/mL)
DMSO	52.7
Distilled H_2O	13.7-14.0
0.1 N HCL	27.7-28.0
0.1 N NaOH	42.0-43.8
35% Ethyl alcohol	14.2-15.0

Stability:

Bulk:

Samples of 5-azacitidine and 5-azacitidine hydrate were found to be stable at 25 °C and 60 °C for at least 30 days.

Solution:

Dilute aqueous solutions of 5-azacitidine have been found to be unstable at 24-26 °C. A 1% aqueous solution at 5-6 °C decomposes 2, 5, and 9% in 2, 8, and 24 hours respectively. At room temperature a 1% aqueous solution shows 7, 20 and 41% decomposition in 2, 8, and 24 hours respectively (UV and NMR).

Ultraviolet Absorption:

(0.1 M acetate buffer, pH 5)

λ_{max} = 242 ± 2 nm ε = 6,850 - 7,250

High Performance Liquid Chromatography:

Column:	Alltech C_8 300 mm x 4.6 mm i.d.
Mobile Phase:	pH 6.5, 0.02 M KH_2PO_4
Flow Rate:	1.5 mL/min
Detection:	UV at 210 nm
Sample Preparation:	0.5 mg of the sample is

	quickly dissolved in 1.0 mL of the mobile phase or internal standard solution
Internal Standard:	Uridine (1.5 mg/mL in mobile phase)
Retention Volume:	6.8 mL (NSC - 102816) 9.0 mL (I.S)

Optical Rotation:

(c = 1, H_2O) $[\alpha]_D^{20} = 40.0 \pm 1.0°$

Toxicity Data:

Woman(iv): TD_{Lo}: 500 μg/kg
Cancer Chemotherapy Reports, 56,413,(1972)

Mouse(po): LD_{50}: 572 mg/kg
Toxicology and Applied Pharmacology, 19,382,(1971)

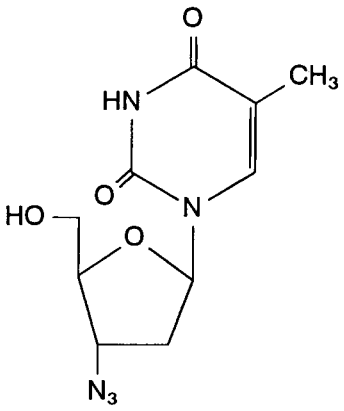
Mouse(ip): LD_{50}: 68 mg/kg
Experientia, 22,53,(1966)

Mouse(iv): LD_{50}: 229 mg/kg
National Technical Information Service, PB84-211432

Dog(iv): LD_{50}: 7200 μg/kg
Advances in Pharmacology and Chemotherapy, 14,285,(1977)

AZT

NSC - 602670



Chemical Name:
3′-Azido-3′-deoxythymidine

Other Names:
Zidovudine; Azidothymidine; Retrovir®; BWA509U

CAS Registry Number: 30516-87-1

Molecular Formula: $C_{10}H_{13}N_5O_4$ **M.W.:** 267.28

Approximate Solubility:	(mg/mL)
Water	15
Ethanol	> 20
DMSO	> 20

Stability:

Bulk:
AZT is stable, as the bulk, at 60 °C for at least 24 hr.
AZT is stable indefinitely at room temperature (25 °C).

Solution:
AZT is stable in DMSO at 45 °C for at least 20 hr.

High Performance Liquid Chromatography:

Column:	IBM Cyano, 250 x 4.6 mm
Mobile Phase:	1% Acetonitrile in water
Flow Rate:	1.0 mL/min
Detection:	UV, 254 nm at 0.1 AUFS
Sample Preparation:	Accurately weighed 1.0 mg samples are each dissolved in 1.00 mL of internal standard solution.
Internal Standard:	Adenosine (1mg/mL).
Retention Volume:	7.4 mL (NSC 602670) 13.5 mL (I.S.)

Optical Rotation:

(c = 1, H_2O) $[\alpha]_D^{20} = +49.0 \pm 0.9°$ (t=21)

Toxicity Data:

Male rat(po): LD50 = 3.1 g/kg
Burroughs Wellcome Company

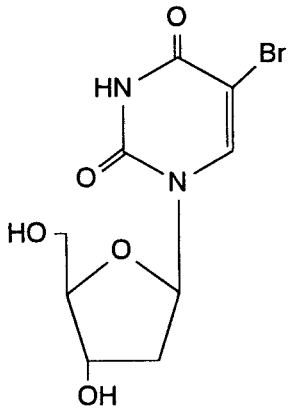
Female rat(po): LD50 = 3.7 g/kg
Burroughs Wellcome Company

Male mice: LD50 = 3.6 g/kg
Burroughs Wellcome Company

Female mice(po): LD50 = 3.1 g/kg
Burroughs Wellcome Company

BROMODEOXYURIDINE

NSC - 38297



Chemical Name:
5-Bromo-2′-deoxyuridine

Other Names:

BUdR; Broxuridine (INN)

CAS Registry Number: 59-14-3

Molecular Formula: $C_9H_{11}N_2O_5Br$ **M.W.:** 307.1

Approximate Solubility:	(mg/mL)
Water	10 - 20
Dimethylacetamide	~ 200
1 N NaOH	> 400
Dimethylsulfoxide	~ 160
Acetone	~ 4

Stability:

Bulk:
The bulk drug should be stored in tightly closed containers at controlled room temperature.

Solution:
BUdR solutions (0.5 and 25 mg/mL) are stable for at least seven days at room temperature.

Ultraviolet Absorption:

(0.1 N HCL)

λ_{max} 280 ± 2 nm ε = 8,900 - 9,400

High Performance Liquid Chromatography:

Column:	30 cm x 3.2 mm Spherisorb ODS
Mobile Phase:	6% MeOH/0.1 M phosphate buffer, pH 5.5
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	1 mg/2 mL in water or internal standard solution
Internal Standard:	benzoic acid (0.8 mg/mL in water)
Retention Volume:	15.0 mL (NSC - 38297) 7.0 mL (I.S.)

Optical Rotation:

(c = 1, 0.1 N NaOH) $[\alpha]_D^{20} = +31 \pm 1°$

Toxicity Data:

Rat(po): LD_{50}: 8400 mg/kg
Iyakuhin Kenkyu, 4,467,(1973)

Rat(ip): LD_{50}: 1500 mg/kg
Advances in Teratology, 3,181,(1968)

Rat(sc): LD_{50}: 3900 mg/kg
Takeda Kenkyusho Ho, 30,530,(1971)

Rat(iv): LD_{50}: 2320 mg/kg
Takeda Kenkyusho Ho, 30,735,(1971)

Mouse(po): LD_{50}: 9100 mg/kg
Takeda Kenkyusho Ho, 30,530,(1971)

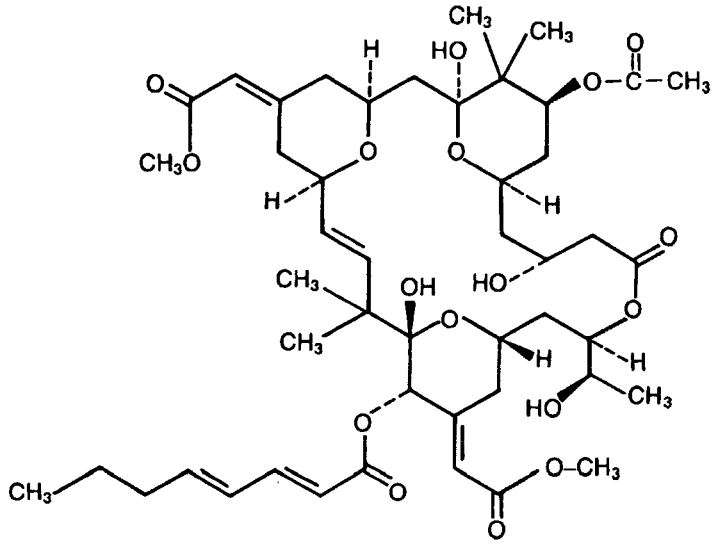
Mouse(ip): LD_{50}: 3050 mg/kg
Takeda Kenkyusho Ho, 30,530,(1971)

Mouse(sc): LD_{50}: 3500 mg/kg
Takeda Kenkyusho Ho, 30,530,(1971)

Mouse(iv): LD_{50}: 2500 mg/kg
Takeda Kenkyusho Ho, 30,530,(1971)

BRYOSTATIN

NSC - 339555



CAS Registry Number: 83314-01-6

Molecular Formula: $C_{47}H_{68}O_{17}$ **M.W.:**905

Approximate Solubility: (mg/mL)

t-Butanol	> 9.2
50% Butanol/water	> 3.0
PET solvent*	> 2.8
Soybean oil	1.5 - 3.0

*PEG 400 (60mL)/EtOH (30mL)/Tween 80 (10 mL)

Stability:

Solution:
Samples dissolved in PET solvent and t-Butanol showed no degradation after storage for 24 and 48 hr at ambient temperature. Samples dissolved in these same solvents showed no degradation after storage at 50 °C for 23 hr.

Ultraviolet Absorption:

(95% ethanol)

λ_{max}	ε
234 ± 2 nm	30,300 ± 100
262 ± 2nm	300 ± 100

High Performance Liquid Chromatography:

Column:	Chemcosorb ODS, 5 μm, 4.6 x 250 mm
Mobile Phase:	80% acetonitrile/20 % water
Flow Rate:	1 mL/min
Detection:	HP 1040 photodiode array detector at 265 nm
Sample Preparation:	0.1 mg dissolved in 0.1 mL ethanol.
Retention Volume:	19.9 mL

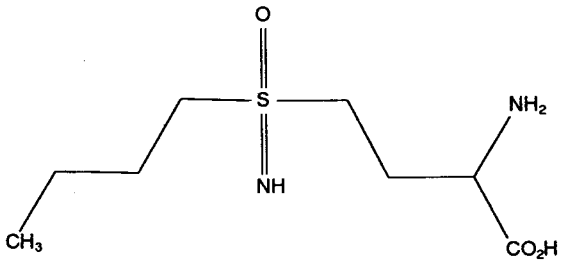
Toxicity Data:

Mouse(iv): LD_{50}: 0.075 mg/kg
Cancer Research Council Data

Rat(iv): LD_{50}: 0.068 mg/kg
Cancer Research Council Data

BSO

NSC - 326231



Chemical Name:
2-amino-4-(*S*-butylsulfonimidoyl)-*L*-butanoic acid

Other Names:
L-Buthionine sulfoximine

CAS Registry Number: 83730-53-4

Molecular Formula: $C_8H_{18}N_2O_3S$ **M.W.:** 222.3

Approximate Solubility:

	(mg/mL)
H_2O	> 100
Acetate buffer, pH4	> 100
Carbonate buffer, pH9	> 100
0.1 N HCl	> 100
0.1 N NaOH	> 100
MeOH	< 1
EtOH (95%)	< 1
CH_3CN	< 1
EtOAC	< 1
$CHCl_3$	< 1
Dimethylacetamide	< 1
DMSO	< 1

Stability:

Bulk:
Samples subjected to both light and dark conditions at room temperature showed no decomposition after 90 days. Samples kept at 50 °C in both light and dark conditions showed about 1% decomposition after 90 days.

Solution:
BSO was found to be stable in aqueous solution for 72 hours when stored at room temperature and under laboratory light.

Ultraviolet Absorption:

(H_2O)

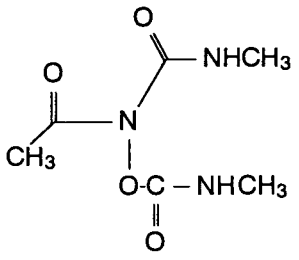
No absorbance was observed between 220-420 nm.

High Performance Liquid Chromatography:

Column:	Alltech Econosphere C_{18}, 5μ 250 x 4.6 mm i.d.
Mobile Phase:	0.01 M Phosphate buffer, pH 5.0
Flow Rate:	1.0 mL/min
Detection:	UV at 205 nm
Sample Preparation:	Samples were prepared in distilled H_2O to give concentrations of approximately 0.57 mg/mL.
Internal Standard:	Thymine (0.003 mg/mL in distilled H_2O)
Retention Volume:	9.95 mL (NSC-326231) 14.3 mL (I.S.)
Optical Rotation:	
(c = 1, 1 N HCl)	$[\alpha]_D^{20} = +32.5 \pm 2°$

CARACEMIDE

NSC - 253272



Chemical Name:
N-Acetyl-*N*-(methylcarbamoyloxy)-*N'*-methylurea

CAS Registry Number: 81424-67-1

Molecular Formula: $C_6H_{11}N_3O_4$ **M.W.:** 189.2

Approximate Solubility: (mg/mL)

H_2O	> 76
Methanol	> 100
Chloroform	> 100

Stability:

Bulk:
The half life at 45 °C is estimated at 8 weeks and the time for 10% decomposition is 2 weeks. The compound is stable at room temperature for 4 weeks (HPLC).

Solution:
A 50 mg/mL solution in water at room temperature showed 5% decomposition after 4 hours and 17% decomposition after 24 hours (HPLC).

Ultraviolet Absorption:

(0.1 N HCl)

The spectrum shows end absorption only.

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 300 x 3.9 mm i.d.
Mobile Phase:	20% CH_3OH in H_2O
Flow Rate:	1.0 mL/min
Detection:	UV at 210 nm
Sample Preparation:	0.5 mg/mL in internal standard solution
Internal Standard:	0.05 mg aniline in 100 mL methanol
Retention Volume:	6.0 mL (NSC-253272) 10.0 mL (I.S.)

Toxicity Data:

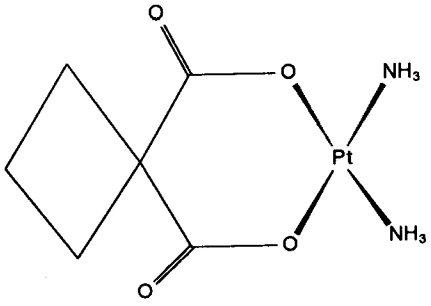
Mouse(po): LD_{50}: 388 mg/kg
NCI Screening Program Data Summary

Mouse(ip): LD_{50}: 167 mg/kg
NCI Screening Program Data Summary

Mouse(iv): LD_{50}: 238 mg/kg
National Technical Information Service, PB84-152032

CARBOPLATIN

NSC - 241240



Chemical Name:
Diammine[1,1-cyclobutanedicarboxylato-(2-)-*O*,*O*']platinum(II), (*SP*-4-2)-

Other Names: CBDCA; Paraplatin; JM-8

Molecular Formula: $C_6H_{12}N_2O_4Pt$ **M.W.:** 371.3

Approximate Solubility:	(mg/mL)
Water	> 15
pH 4 Acetate Buffer	5 - 10
pH 9 Carbonate Buffer	5 - 10
10% Ethanol/H_2O	5 - 10
95% Ethanol/H_2O	< 1
0.1 N HCl	5 - 10
0.1 N NaOH	5 - 10
Methanol	< 1
Chloroform	< 5
Dimethylsulfoxide	5
Acetic Acid	< 1
Trifluoroacetic Acid	< 1

Stability:

Bulk:
No decomposition was detected after 30 days at 60 °C in the dark (HPLC).

Solution:
After 48 hours at room temperature an aqueous solution showed < 1% decomposition (HPLC).

High Performance Liquid Chromatography:

Column:	Unimetrics LiChrosorb RP -8, 250 x 4.6 mm i.d.
Mobile Phase:	Water
Flow Rate:	1.0 mL/min
Detection:	UV at 205 nm
Sample Preparation:	0.6 mg/mL in water
Internal Standard:	(0.11 mg uracil/mL water)
Retention Volume:	6.2 mL (NSC-241240) 5.5 mL (I.S.)

Toxicity Data:

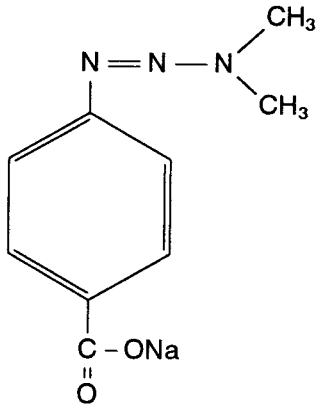
Rat(iv): LD_{50}: 61 mg/kg
Journal of the National Cancer Institute, 67,201,(1981)

Mouse(ip): LD_{Lo}: 150 mg/kg
Bioinorganic Chemistry,2,187,(1973)

Mouse(iv): LD_{50}: 143 mg/kg
National Technical Information Service, PB82-165028

CB 10-277

NSC - 208107



Chemical Name:
4-(3,3-Dimethyl-1-triazenyl)benzoic acid, sodium salt

CAS Registry Number: 49638-52-0

Molecular Formula: $C_9H_{10}N_3O_2Na$ **M.W.**:215.1

Approximate Solubility:	(mg/mL)
Water	> 50
Acetate buffer, pH 4	<1
Carbonate buffer, pH 9	> 50
0.1 N HCl	1
Ethanol	16
Methanol	> 50
Dimethyl acetamide	< 1
DMSO	3

DMF	1
Acetonitrile	< 1
Ethyl acetate	< 1
Chloroform	< 1
Toluene	< 1

Stability:

Bulk:
No significant decomposition was observed after 90 days storage at room temperature and at 50 °C under light and dark conditions.

Solution:
The compound was determined to be unstable in distilled water through 72 hr when stored at room temperature under normal laboratory light. The t_{90} was calculated as 28.56 hr.

Ultraviolet Absorption:

(MeOH)

λ_{max}	ε
318 ± 2 nm	19,860 ± 110

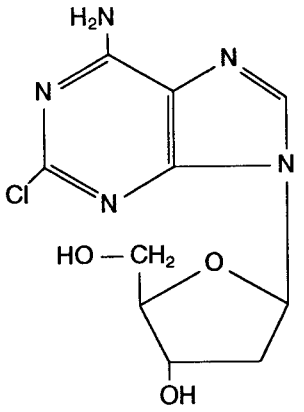
High Performance Liquid Chromatography:

Column:	Alltech Econosphere, 5 μ, 250 x 4.6 mm i.d.

Mobile Phase:	Methanol/1% Acetic Acid (50/50, v/v)
Flow Rate:	1.0 mL/min
Detection:	313 nm
Sample Preparation:	≈0.625 and 0.025 mg/mL in methanol
Internal Standard:	*p*-Aminobenzoic acid, 0.6208 mg/mL in methanol
Retention Volume:	13.5 mL (NSC 208107) 3.5 mL (I.S.)

2-CHLORO-2'-DEOXYADENOSINE

NSC - 105014



CAS Registry #: 4291-63-8

Molecular Formula: $C_{10}H_{12}ClN_5O_3$ **M.W.:** 286

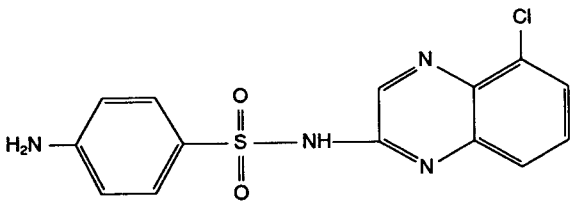
High Performance Liquid Chromatography:

Column:	Alltech C_8, 25 cm x 4.6 mm
Mobile Phase:	10% acetonitrile in pH 5.5, 0.05M $NH_4H_2PO_4$
Flow Rate:	1.0 mL/min
Detection:	UV at 265 nm
Sample Preparation:	1 mg samples dissolved in 10 mL of internal standard solution

Internal Standard:	1 mg orcinol/mL MeOH
Retention Volume:	11.6 mL (NSC 105014) 14.1 mL (I.S.)

CHLOROSULFAQUINOXALINE

NSC - 339004



Chemical Name:
4-Amino-*N*-[5-chloro-2-quinoxalinyl]benzenesulfonamide

Other Names:
Chloroquinoxaline; CSQ

CAS Registry Number: 97919-22-7

Molecular Formula: $C_{14}H_{11}ClN_4O_2S$ **M.W.:** 334.8

Approximate Solubility:	(mg/mL)
H_2O	< 1
pH 4 Acetate buffer	< 1
pH 9 Carbonate buffer	10 - 12
0.1 N HCl	< 1
0.1N NaOH	≈ 25 - 30
MeOH	5 - 7
EtOH (95%)	4 - 6
DMSO	> 50

Stability:

Bulk:
The compound is stable at room temperature and ordinary laboratory illumination for at least 90 days. In a capped glass vial and heated at 50 °C, the compound is stable for at least 90 days (HPLC).

Solution:
Dilute solutions (0.8 mg/mL) in 50% DMSO were stable for up to 72 hours (UV).

Ultraviolet Absorption:

λ_{max}	ε
339 ± 2 nm	5,820 ± 300
269 ± 2 nm	26,730 ± 1,200
255 ± 2 nm	31,000 ± 2,200

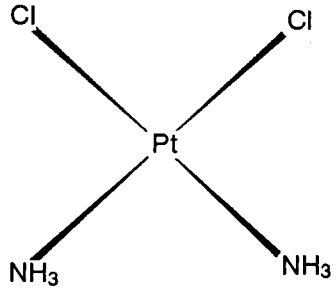
High Performance Liquid Chromatography:

Column:	Alltech Econosphere C_{18}, 5μ, 250 x 4.6 mm i.d.
Mobile Phase:	CH_3CN/water containing 0.005 M heptanesulfonic acid and sulfuric acid to adjust pH to 3.0, 30/70, v/v.
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm

Sample Preparation:	0.08 mg/mL in CH_3CN
Internal Standard:	Propriophenone, 0.1 mg/mL
Retention Volume:	15.8 mL (NSC-339004) 18.2 mL (I.S.)

CISPLATIN

NSC - 119875



Chemical Name:
Diamminedichloroplatinum, *cis*-

Other Names:
cis-Diamminedichloroplatinum (II); CDP; DDP; Cisplatin (USAN)

CAS Registry Number: 15663-27-1

Molecular Formula: $PtCl_2H_6N_2$ **M.W.:** 300.1

Approximate Solubility:	(mg/mL)
H_2O	1
DMSO	10
10:1 PVP coprecipitate in 10% PVP	2.5
Dimethylformamide (pure anhydrous)	24

Stability:

Solution:
Aqueous solutions decompose in two steps to a compound that has two water molecules replacing the two chlorine atoms. At 30 °C the half life is five hours at neutral pH. The platinum compound is attacked by a variety of nucleophiles (i.e. hydroxide ion, pyridine, nitrate ion) which replace the chlorine atoms.

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max} = 301 ± 2 nm ε = 124 - 145

High Performance Liquid Chromatography:

Column:	250 mm x 4 mm i.d. Zorbax NH_2
Mobile Phase:	5% H_2O in absolute EtOH
Flow Rate:	2.5 mL/min
Detection:	UV at 210 nm
Sample Preparation:	1 mg/mL in 0.1 N HCL or internal standard solution
Internal Standard:	guanosine (0.6 mg/mL in 0.1 N HCL)
Retention Volume:	30 mL (NSC - 119875) 17.5 mL (I.S.)

Toxicity Data:

Human(iv): TD_{Lo}: 2500 μg/kg
Cancer Chemotherapy Reports, 59,647,(1975)

Rat(po): LD_{50}: 25800 μg/kg
Yakuri to Chiryo. Pharmacology and Therapeutics, 10,723,(1982)

Rat(ip): LD_{50}: 8300 μg/kg
Kiso to Rinsho. Clinical Report, 15,5669,(1981)

Rat(sc): LD_{50}: 8100 μg/kg
Kiso to Rinsho. Clinical Report, 15,5669,(1981)

Rat(iv): LD_{50}: 8 mg/kg
Journal of the National Cancer Institute, 67,201,(1981)

Rat(im): LD_{50}: 9200 μg/kg
Yakuri to Chiryo. Pharmacology and Therapeutics, 10,723,(1982)

Mouse(po): LD_{50}: 32700 μg/kg
Kiso to Rinsho. Clinical Report, 15,5669,(1981)

Mouse(ip): LD_{50}: 17400 μg/kg
Kiso to Rinsho. Clinical Report, 15,5669,(1981)

Mouse(sc): LD_{50}: 16900 μg/kg
Yakuri to Chiryo. Pharmacology and Therapeutics, 10,723,(1982)

Mouse(iv): LD_{50}: 12 mg/kg
Toxicology and Applied Pharmacology, 25,230,(1973)

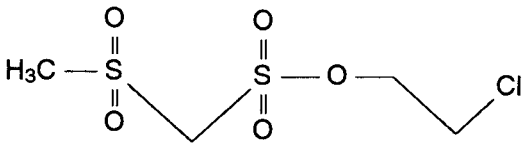
Mouse(im): LD_{50}: 17900 μg/kg
Yakuri to Chiryo. Pharmacology and Therapeutics, 10,723,(1982)

Dog(iv): LD_{50}: 2500 μg/kg
Toxicology and Applied Pharmacology, 25,230,(1973)

Monkey(iv): LD_{50}: 250 μg/kg
Cancer, 33,1219,(1974)

CLOMESONE

NSC - 338947



Chemical Name:
Methylsulfonylmethanesulfonic acid, 2-chlorethyl ester

CAS Registry Number: 88343-72-0

Molecular Formula: $C_4H_9ClO_5S_2$ **M.W.:** 236.7

Approximate Solubility: (mg/mL)

Water	4
Acetate buffer, pH 4	6
Carbonate buffer, pH 9	6
0.1 N HCl	4
0.1 N Naoh	15
Ethanol (95%)	18
Methanol	> 50
Acetonitrile	> 50
DMSO	> 50

Stability:

Bulk:

Clomesone is stable at room temperature in light or dark conditions but is unstable when stored at 50 °C in both light and dark conditions.

Solution:

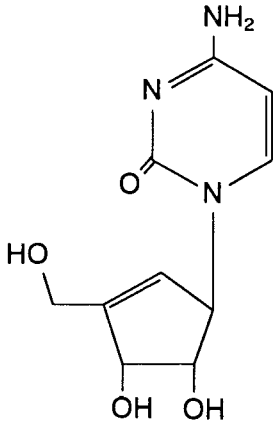
The t_{90} of an aqueous solution is 207 minutes.

High Performance Liquid Chromatography:

Column:	Altex Ultrasphere ODS, 5μ, 250 x 4.6 mm i.d.
Mobile Phase:	CH_3CN/0.067 M phosphate buffer, pH 7.0 (25/75, v/v)
Flow Rate:	1.0 mL/min
Detection:	Refractive index
Sample Preparation:	Sample was dissolved in mobile phase.
Internal Standard:	acetophenone, 0.26 μL/mL
Retention Volume:	9.5 mL (NSC 338947) 19.9 mL (I.S.)

CYCLOPENTENYLCYTOSINE

NSC - 375575



Chemical Name: 4-Amino-1-[4,5- dihydroxy-3-(hydroxymethyl)-2-cyclopenten-1-yl]-2(1*H*)-pyrimidinone, (1*R*-(1α,4β,5β))-

Other Name:
CPE-C

CAS Registry Number: 90597-22-1

Molecular Formula: $C_{10}H_{13}N_3O_4$ **M.W.:239.2**

Approximate Solubility:	(mg/mL)
Water	7.5
Acetate buffer, pH 4	10.0
Carbonate buffer, pH 9	7.5
0.1 N HCl	15.0
0.1 N NaOH	7.5
Ethanol	< 1
Methanol	< 1

Butanol	< 1
Dimethylacetamide	> 30.0
DMSO	> 30.0
Acetonitrile	< 1
Ethyl acetate	< 1
Chloroform	< 1
Toluene	< 1

Stability:

Bulk:

CPE-C was found to be stable under the following conditions: room temperature, dark; room temperature, light; 50 °C, dark; 50 °C, light.

Solution:

CPE-C was found to be stable at room temperature in 0.9% saline over a 75 hr period under exposure to light.

Ultraviolet Absorption:

(H_2O)

λ_{max} = 275 ± 2nm ε = 9708 ± 184

High Performance Liquid Chromatography:

Column:	Beckman Ultrasphere, 5μ, 4.6 x 250 mm
Mobile Phase:	Methanol: 5 mM heptanesulfonic acid (20:80) adjusted to pH 3.2 with sulfuric acid

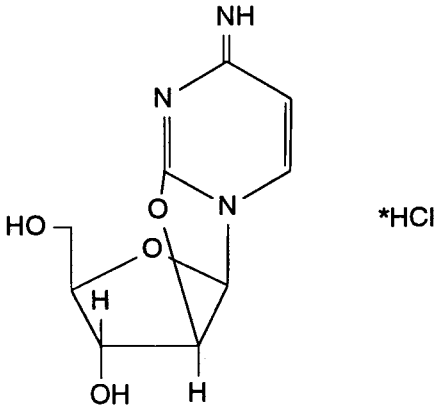
Flow Rate:	1.0 mL/min
Detection:	280 nm, 0.5 AUFS
Sample Preparation:	20 μL of 0.12 mg/mL solution in mobile phase
Internal Standard:	phenol, 2 μL/mL in mobile phase
Retention Volume:	16 mL (NSC 375575) 26 mL (I.S.)

Optical Rotation:

(c = 0.3,0.1M phosphate buffer) $[\alpha]_D^{23} = -95 \pm 5°$

CYCLOCYTIDINE HYDROCHLORIDE

NSC - 145668



Chemical Name:
2,3,3a,9a-Tetrahydro-3-hydroxy-6-imino6*H*-furo(2′,3′:4,5)-oxazolo(3,2-*a*)pyrimidine-2-methanol,-,monohydrochloride

Other Names:
Cyclo-C; Cyclocytidine hydrochloride

CAS Registry Number: 10212-25-6

Molecular Formula: $C_9H_{11}N_3O_4 \cdot HCl$ **M.W.:** 261.7

Approximate Solubility: (mg/mL)

H_2O	200
EtOAc	< 0.1
$CHCl_3$	< 0.1

Stability:

Bulk:

A sample stored at 60 °C for 30 days showed no decomposition as indicated by optical rotation.

Solution:

A 1% solution in water after 24 hours at room temperature showed no decomposition as indicated by optical rotation.

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 300 x 3.9 mm i.d.
Mobile Phase:	1.5% acetic acid in water with 0.075 M heptanesulfonic acid
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	Sample concentration - 1.0 mg/mL
Retention Volume:	8.2 mL (NSC - 145668)

Ultraviolet Absorption:

(H_2O)

λ_{max}	ε
231 ± 2 nm	9,300 - 9,700
263 ± 2 nm	10,400 - 10,800

Optical Rotation:

($c=2$, H_2O) $[\alpha]_D^{20} = -22 \pm 2°$

Toxicity Data:

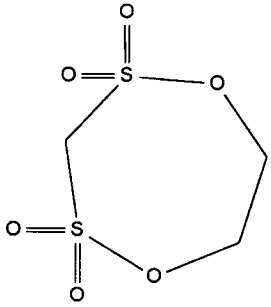
Mouse(iv): LD_{50}: 800 mg/kg
Drugs in Japan. Ethical Drugs, 6,55,(1982)

Dog(iv): LD_{50}: 344 mg/kg
Oyo Yakuri, Pharmacometrics, 8,353,(1974)

Monkey (iv): LD_{50}: 1045 mg/kg
Oyo Yakuri. Pharmacometrics, 8,353,(1974)

CYCLODISONE

NSC - 348948



Chemical Name:
1,5,2,4-Dioxadithiepane, 2,2,4,4-tetraoxide

Other Names: Cyclic-SOSO

CAS Registry Number: 99591-73-8

Molecular Formula: $C_3H_6O_6S_2$ **M.W.:** 202.2

Approximate Solubility: (mg/mL)

Water	< 1
Acetate buffer, pH 4	< 1
Carbonate buffer, pH 9	< 1
0.1 N HCl	< 1
0.1 N NaOH	10-13
Ethanol (95%)	< 1
Acetone	> 100
CH_3CN	> 100
$CHCl_3$	< 1
DMSO	> 100
DMF	> 100

Stability:

Bulk:

Cyclodisone stored for 90 days at room temperature and at 50 °C under both dark and light conditions was stable (HPLC). Samples stored at 50 °C turned a light tan color.

Solution:

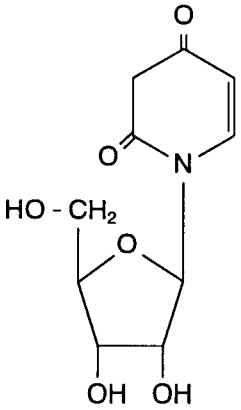
180 mg of Cyclodisone was dissolved in 60 mL of DMSO/water (50/50, v/v). Aliquots of this solution (5 mL) were diluted to 10 mL with internal standard solution (5 mL, phenol 1.8 mg/mL in CH_3CN/water, 20/80, v/v) and the concentration was determined over a 4 hour period using the HPLC system described below. The t_{90} was 320 min.

High Performance Liquid Chromatography:

Column:	Altech Ultrasphere ODS, 5μ, 250 x 4.6 mm i.d.
Mobile Phase:	CH_3CN/water (20/80,v/v)
Flow Rate:	1.0 mL/min
Detection:	Refractive index
Sample Preparation:	1.7 mg/mL in CH_3CN/H_2O (20/80,v/v)
Internal Standard:	Phenol, 1.8 mg/mL
Retention Volume:	7.5 mL (NSC 348948) 12.5 mL (I.S.)

3-DEAZAURIDINE

NSC - 126849



Chemical Name:
1-β-*D*-ribofuranosyl-2,4(1*H*,3*H*)-pyridinedione

CAS Registry Number: 39935-49-4

Molecular Formula: $C_{10}H_{13}NO_6$ **M.W.:** 243.2

Approximate Solubility:	(mg/mL)
H_2O	18
DMSO	> 150
EtOH	< 1
DMF	> 150
EtOAc	0.2
$CHCl_3$	0.2

Stability:

Bulk:
A sample stored at 60 °C for 30 days showed no decomposition by UV absorption or paper chromatography.

Solution:
A 2% aqueous solution held at room temperature for 24 hours showed no decomposition by UV absorption or paper chromatography.

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{max} = 255 ± 2 nm ε = 7,850 - 8,200

High Performance Liquid Chromatography:

Column:	Altex Ultrasphere, 5μ, 250 x 4.6 mm i.d.
Mobile Phase:	Methanol/0.1 M acetate buffer, pH 4 (3:97)
Flow Rate:	1 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.2 mg/mL in mobile phase
Internal Standard:	Thymidine, 0.06 mg/mL in mobile phase

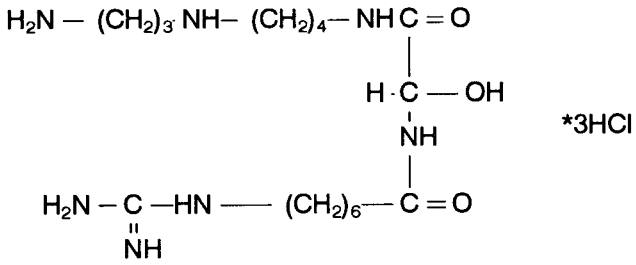
Retention Volume: 9.6 mL (NSC - 126849)
18.7 mL (I.S)

Optical Rotation:

(c = 1, H_2O) $[\alpha]_D^{20} = 43 \pm 2°$

DEOXYSPERGUALIN

NSC - 356894



Chemical Name:
7-[(Aminoiminomethyl)amino]-*N*-[2-[[4-[(3-amino-propyl)amino]butyl]amino]-1-hydroxy-2-oxoethyl]heptanamide,(+)-trihydrochloride

Other Names:
15-Deoxyspergualin trihydrochloride

CAS Registry Number: 114760-38-2

Molecular Formula: $C_{17}H_{37}N_7O_3 \cdot 3HCl$ **M.W.:** 496.9

Approximate Solubility:	(mg/mL)
H_2O	> 100
0.1N NaOH	> 100
0.1N HCl	> 100
95% EtOH	> 100

MeOH	> 100
DMSO	> 100
$CHCl_3$	< 0.2

Stability:

Bulk:

Samples stored at 25 °C for 3 months show 5-8% decomposition (HPLC).

Solution:

As a 2 mg/mL solution in water at 25 °C, 15-deoxyspergualin is stable for at least 28 hrs under ordinary laboratory conditions (HPLC).

Ultraviolet Absorption:

(95% EtOH)

The spectrum shows end absorption only.

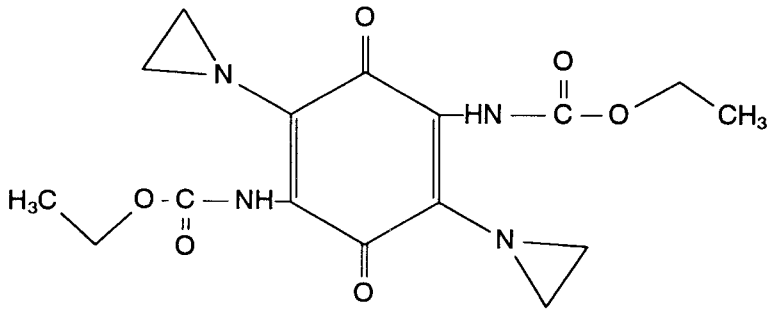
High Performance Liquid Chromatography:

Column:	Ultrasphere ODS, 220 x 4.6 mm i.d.
Mobile Phase:	10% CH_3CN in 0.1 M KH_2PO_4 and 0.005 M hexanesulfonic acid sodium salt, pH adjusted to 3 with H_3PO_4
Flow Rate:	1.0 mL/min
Detection:	UV at 205 nm

Sample Preparation:	Approximately 1 mg/mL in water.
Internal Standard:	2-naphthalenesulfonic acid, 4mg/25 mL water.
Retention Volume:	15.7 mL (NSC-356894) 10.4 mL (I.S.)

DIAZIQUONE

NSC - 182986



Chemical Name:
2,5-Bis(1-aziridinyl)-3,6-dioxo-1,4-cyclohexadiene-1,4-dicarbamic acid, diethyl ester

Other Names:
AZQ; Aziridinylbenzoquinone

CAS Registry Number: 57998-68-2

Molecular Formula: $C_{16}H_{20}N_4O_6$ **M.W.:** 364.4

Approximate Solubility:	(mg/mL)
Water	0.72
pH 4 buffer	< 1
pH 9 buffer	< 1
10% Ethanol	< 1
95% Ethanol	< 1
Methanol	< 1

Chloroform	5 - 7
5% Dimethylacetamide	1.5
Dimethylacetamide	20 - 25
Dimethylsulfoxide	25 - 30

Stability:

Bulk:
A sample stored at 60 °C in the dark for 30 days showed < 2% decomposition (HPLC).

Solution:
A sample in 5% DMA (1mg/mL) showed 18% decomposition after 8 hours at room temperature. (HPLC)

Ultraviolet Absorption:

(Methanol)

λ_{max}	ε
217 ± 2 nm	22,000 - 22,800
341 ± 2 nm	13,900 - 14,300

High Performance Liquid Chromatography:

Column:	μ–Bondapak Phenyl, 300 x 4 mm i.d.
Mobile Phase:	CH_3CN/0.01 M pH 7 phosphate, 15/85, v/v
Flow Rate:	1.0 mL/min

Detection: UV at 254 nm

Sample Preparation: Sample solvent CH_3CN

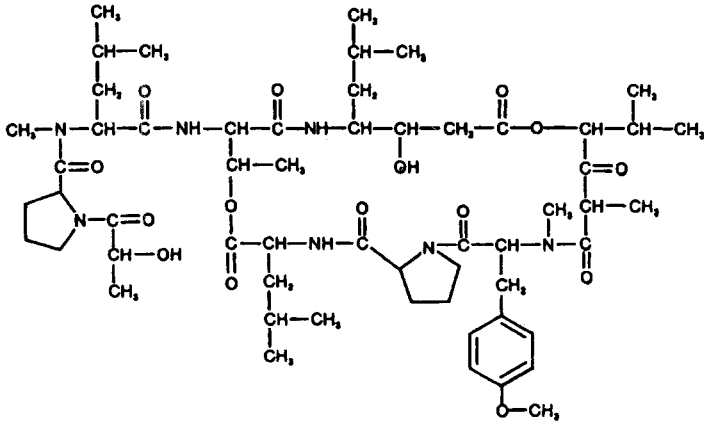
Retention Volume: 15 mL (NSC-182986)

Toxicity Data:

Mouse(iv): LD_{50}: 10300 μg/kg
National Technical Information Service, PB80-177934

DIDEMNIN B

NSC - 325319



Chemical Name: *N*-[1-[*N*-[4-[[3-Hydroxy-4-[[*N*-[*N*-[1-(2-hydroxy-1-oxopropyl)-*L*-prolyl]-*N*-methyl-*L*-leucyl]-*L*-threonyl]amino-5-methyl-1-oxoheptyl]oxy]-2,5-dimethyl-1,3-dioxohexyl]-*L*-leucyl]-*L*-prolyl]-*N*,*O*-dimethyl-*L*-tyrosine, ϕ-lactone

CAS Registry Number: 77327-05-0

Molecular Formula: $C_{57}H_{89}N_7O_{15}$ **M.W.:** 1112.0

Approximate Solubility:	(mg/mL)
H_2O	< 0.1
CH_3OH	> 100
$CHCl_3$	> 100
DMSO	> 100
C_2H_5OH	> 100
CH_2Cl_2	> 100

Stability:

Bulk:
As a bulk chemical, didemnin B is found to be stable at 25 ± 2 °C for 3 weeks. At the end of 4 weeks, approximately 2% decomposition has occurred.
When stored at 45 °C, didemnin B appeared stable for 2 weeks; after this time, it slowly decomposed to an approximate 7% loss at the end of 4 weeks (HPLC).

Solution:
As a 6 mg/mL 50% aqueous ethanol solution at room temperature (25 ± 2 °C) didemnin B appeared stable for at least 26 hours (HPLC).

Ultraviolet Absorption:

(MeOH)

λ_{max}	ε
284 ± 2 nm(sh)	1,455 - 1,490
277 ± 2 nm	1,705 - 1,750
220 ± 2 nm(sh)	17,500 - 19,199
205 ± 2 nm	29,100 - 29,700

High Performance Liquid Chromatography:

Column:	Whatman Partisil 5 ODS, 250 mm x 4.6 mm i.d.
Mobile Phase:	CH_3OH/H_2O/triethylamine, 75/25/0.01 (adjusted to pH 7.5 with acetic acid)

Flow Rate:	1.0 mL/min
Detection:	UV at 275 nm
Sample Preparation:	3 mg/mL in internal standard solution
Internal Standard:	1 mL hexaphenone per liter methanol
Retention Volume:	19 mL (NSC-325319) 10 mL (I.S.)

Toxicity Data:

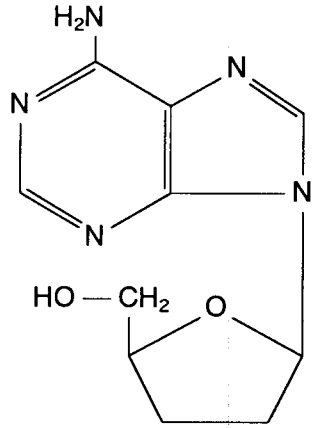
Rat(iv): LD_{50}: 860 μg/kg
National Technical Information Service, PB84-192251

Mouse(iv): LD_{50}: 1530 μg/kg
National Technical Information Service, PB84-192251

Dog (iv): LD50: 418 g/kg
National Technical Information Service, PB84-192251

DIDEOXYADENOSINE

NSC - 98700



Chemical Name: 2′,3′-Dideoxyadenosine

Other Name: DDA

CAS Registry Number: 4097-22-7

Molecular Formula: $C_{10}H_{13}N_5O_2$ **M.W.:** 235.2

Approximate Solubility:	(mg/mL)
H_2O	3.4-5.1
Buffer, pH4	4.8-9.6
Buffer, pH9	3.2-4.8
EtOH	1.6-2.0
DMA	2.6-3.4
DMSO	3.3-5.0
$CHCL_3$	< 0.7
EtOAc	< 0.7
t-BuOH	< 0.7

Stability:

Bulk:
2′,3′-Dideoxyadenosine is stable as a bulk chemical for at least 6 weeks at room temperature and 45 °C, under light or dark conditions.

Solution:
DDA was stable as a 0.1 mg/mL water solution for at least 23 hrs at room temperature.

Ultraviolet Absorption:

(water)

λ_{max}	ε
260 ± 2 nm	14,500 ± 500
208 ± 2 nm	19,500 ± 700

High Performance Liquid Chromatography:

Column:	IBM C_8, 250 x 4.5 mm i.d.
Mobile Phase:	8% CH_3CN in 0.05M $NH_4H_2PO_4$
Flow Rate:	1 mL/min
Detection:	UV at 254 nm
Sample Preparation:	1 mg/10 mL of internal standard solution. Sonicate samples 10 minutes before injection.

Internal Standard: Approx. 4 mg orcinol/mL in MeOH/H_2O (50:50).

Retention Volume: 9.5 mL (NSC 98700)
18.3 mL (I.S.)

Optical Rotation:

(c = 1, H_2O) $[\alpha]_D^{25} = -28 \pm 2°$

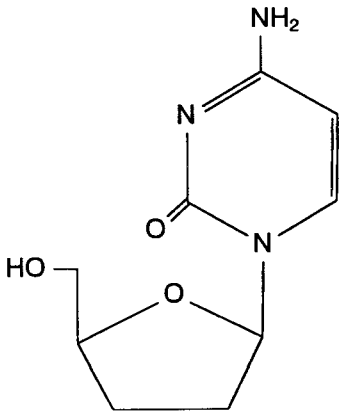
Toxicity Data:

Mouse(po): LD_{50}: 5 gm/kg
Antimicrobial Agents & Chemotherapy, 19,424,(1981)

Mouse(sc): LD_{50}: 1320 mg/kg
Antimicrobial Agents & Chemotherapy, 19,424,(1981)

DIDEOXYCYTIDINE

NSC - 606170



Chemical Name:
2′,3′-Dideoxycytidine

Other Names:
DDC

CAS Registry Number: 7481-89-2

Molecular Formula: $C_9H_{13}N_3O_3$ **M.W.:** 211.2

Approximate Solubility:	(mg/mL)
H_2O (warm)	80-90
Acetate buffer, pH 4	> 50
Carbonate buffer, pH 9	> 50
0.1N HCl	> 50
0.1N NaOH	> 50
EtOH (95%)	5-7

MeOH	8-10
BuOH	< 1
DMA	7-10
DMSO	90-100
DMSO (70%)	50-60
CH_3CN	< 1
EtOAc	< 1
$CHCl_3$	< 1
Toluene	< 1

Stability:

Bulk:
Dideoxycytidine is stable in bulk form through 90 days at room temperature and at 50 °C under both light and dark conditions.

Solution:
Dideoxycytidine was stable in distilled water through 72 hrs.

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max} = 280 ± 2nm ε = 13,300 ± 700

High Performance Liquid Chromatography:

Column:	Alltech Econosphere, 300 x 3.9 mm i.d.
Mobile Phase:	0.2 M Ammonium acetate, pH 7.0
Flow Rate:	1 mL/min

Detection: UV at 280 nm

Sample Preparation: Approximately 10 mg (accurately weighed) is dissolved in 50 mL water. Four mL of this solution is added to 2 mL of internal standard solution and the resulting solution is diluted to 10 mL with distilled water.

Internal Standard: 5-Bromo-2′-deoxyuridine, ≈0.5 mg/mL in methanol.water, 5/45, v/v.

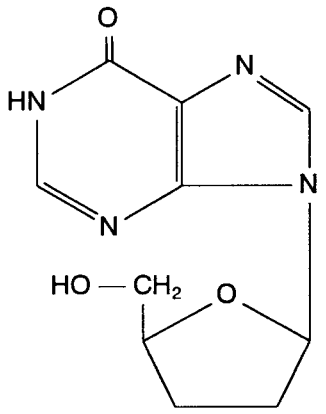
Retention Volume: 37 mL (NSC-606170)
51 mL (I.S.)

Optical Rotation:

(c = 1, H_2O) $[\alpha]_D^{25} \geq +70°$

DIDEOXYINOSINE

NSC - 612049



Chemical Name: 2′,3′- Dideoxyinosine

Other Names: DDI; Didanosine (USAN/INN)

CAS Registry Number: 69655-05-6

Molecular Formula: $C_{10}H_{12}N_4O_3$ **M.W.:** 236.2

Approximate Solubility:	(mg/mL)
H_2O	20
0.1 N KH_2PO_4 (pH4)	19
0.1 N KH_2PO_4 (pH9)	23
MeOH	5
EtOH	2.5
DMSO	43
$CHCl_3$	insoluble

Stability:

Bulk:
The compound is stable for at least 6 weeks at room temperature and 45 °C under both light and dark conditions.

Solution:
The compound is stable as a 0.5 mg/mL aqueous solution for more than 24 hrs under normal laboratory conditions.

Ultraviolet Absorption:

λ_{max}	ε
203 ± 2nm	18,400 - 19,970
249 ± 2nm	12,200 - 12,500

High Performance Liquid Chromatography:

Column:	IBM ODS, 250 x 4.6 mm i.d.
Mobile Phase:	10% MeOH/0.1N KH_2PO_4, pH = 6.8
Flow Rate:	1.3 mL/min

Detection: UV at 254 nm

Sample Preparation: 1 mg DDI dissolved in 2 mL water

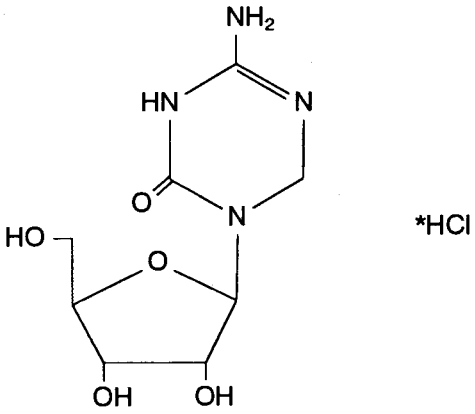
Retention Volume: 14.7 mL

Optical Rotation:

(c = 1, H_2O) $[\alpha]_D^{20} = -25.7 \pm 2°$

DIHYDRO-5-AZACYTIDINE HYDROCHLORIDE

NSC - 264880



Chemical Name:
4-Amino-5,6-dihydro-1-β-*D*-ribofuranosyl-1,3,5-triazin-2(1*H*)-one, monohydrochloride

Other Names:
DHAC

CAS Registry Number: 62402-31-7

Molecular Formula: $C_8H_{14}N_4O_5 \cdot HCl$ **M.W.:** 282.7

Approximate Solubility:	(mg/mL)
H_2O	> 50
pH 4 Acetate buffer	> 50
pH 9 Borate buffer	> 50

10% Ethanol	> 50
95% Ethanol	1 - 3
MeOH	5 - 10
$CHCl_3$	< 1

Stability:

Bulk:
A sample stored at 60 °C for 30 days showed < 1% decomposition (TLC, UV).

Solution:
A sample was dissolved in pH 8 phosphate buffer at a concentration of 0.1 mg/mL for UV study and 10 mg/mL for TLC study and stored at room temperature in a closed clear bottle exposed to laboratory light for 9 days. Based on the UV and TLC the sample showed < 1% decomposition.

Ultraviolet Absorption:

(pH 9 Phosphate Buffer)

λ_{max} = 234 ± 2 nm ε = 6,700 - 7,100

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 300 x 3.9 mm i.d.
Mobile Phase:	Water containing 0.005 M heptane-sulfonic acid and 1% acetic acid (v/v)
Flow Rate:	2 mL/min

Detection: UV at 234 nm

Sample Preparation: 1 mg/mL in mobile phase containing internal standard.

Internal Standard: 0.063 mg/mL guanosine

Retention Volume: 16.6 mL (NSC-264880)

Optical Rotation:

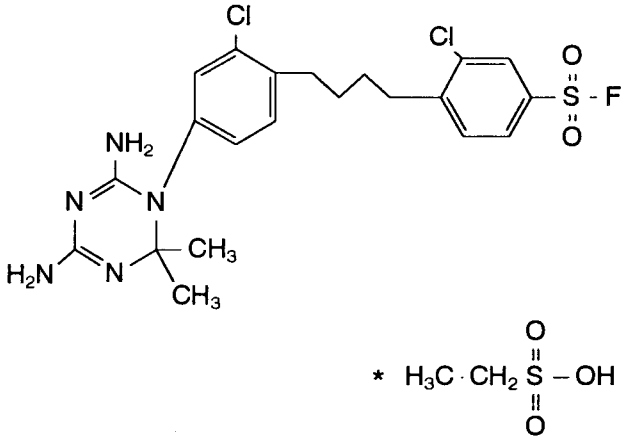
(c = 1.3, H_2O) $[\alpha]_D^{25} = -27.5 \pm 2°$

Toxicity Data:

Mouse(iv): LD_{50}: 2559 mg/kg
National Technical Information Service, PB82-195751

DIHYDROTRIAZINE BENZENESULFONYL FLUORIDE

NSC - 127755



Chemical Name: Ethanesulfonic acid, compd. with 3-chloro-4-(4-(2-chloro-4-(4,6-diamino-2,2-dimethyl-1,3,5-triazin-1-(2*H*)-yl)phenyl)butyl)benzenesulfonyl fluoride (1:1)

Other Names: Triazine antifol

CAS Registry Number: 31368-48-6

Molecular Formula: $C_{21}H_{24}Cl_2FN_5O_2S \cdot C_2H_5SO_3H$ **M.W.:** 610.6

Approximate Solubility:	(mg/mL)
TFA	> 200
DMSO	200
MeOH	35
95% EtOH	9.7
H_2O	0.09
10% DMA	3.3

Stability:

Bulk:
As a bulk chemical kept in a screw-capped vial and stored in a 60 °C oven, the sample appeared stable for at least 30 days (HPLC).

Solution:
A saturated solution in 10% aqueous DMA is stable at room temperature for 24 hours (HPLC).

Ultraviolet Absorption:

(95% EtOH)

λ_{max} = 235 ± 2 nm ε = 22,500 - 23,000

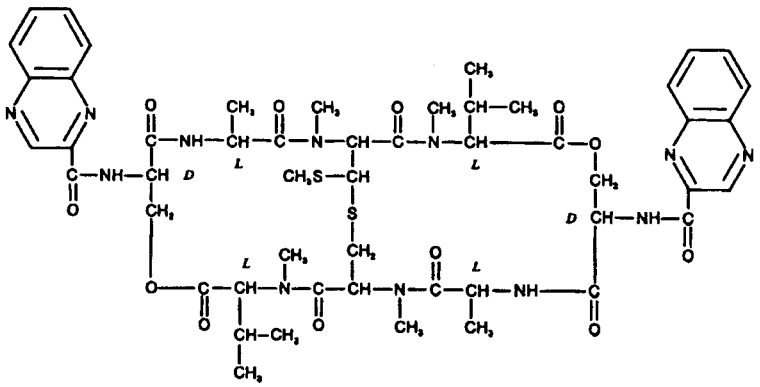
High Performance Liquid Chromatography:

Column:	μPorasil, 28 cm x 3.2 mm i.d.
Mobile Phase:	10% MeOH in CH_2Cl_2 with 4 x 10^{-4} M PIC B-7
Flow Rate:	1 mL/min
Detection:	UV at 254 nm
Sample Preparation:	1 mg/mL in methanol or internal standard solution

Internal Standard:	3,4-diaminobenzoic acid (8 mg/25 mL methanol)
Retention Volume:	22.0 mL (NSC - 127755) 12.5 mL (I.S.)

ECHINOMYCIN

NSC - 526417



Other Name:
Quinomycin A

CAS Registry Number: 512-64-1

Molecular Formula: $C_{51}H_{64}N_{12}O_{12}S_2 \cdot H_2O$ **M.W.:** 1119.3

Approximate Solubility:
Soluble in 5% Cremophor EL/5% ethanol/90% water at 0. 4mg/mL. Very insoluble in water.

Stability:

Bulk:
Should be stored at 5 °C or less.

Ultraviolet Absorption:

(Methanol)

λ_{max}	ε
321 ± 2nm	12,500 - 13,500
243 ± 2nm	73,400 - 77,400

High Performance Liquid Chromatography:

Column: μBondapak C_{18}, 300 x 3.9mm i.d.

Mobile Phase: Acetonitrile/water, 60/40 (v/v)

Flow Rate: 1 mL/min

Detection: UV at 254 nm

Sample Preparation: 0.5 mg/mL in acetonitrile

Retention Volume: 5.8 mL (NSC-526417)

Optical Rotation:

(c = 1.10, chloroform) $[\alpha]_D^{23}$ = -321 ± 2°

Toxicity Data:

Mouse(ip): LD_{50}: 400 μg/kg
Antibiotics: Origin, Nature and Properties, 1,311,(1978)

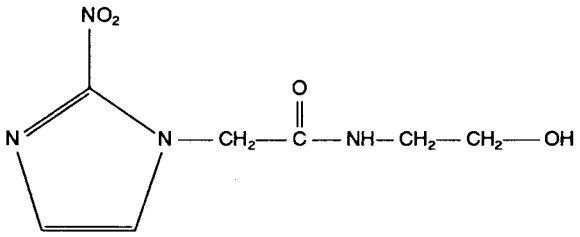
Mouse(sc): LD_{50}: 3800 μg/kg
Antibiotics: Origin, Nature and Properties, 1,311,(1978)

Mouse(iv): LD_{50}: 629 μg/kg
National Technical Information Service, PB83-114298

Dog(iv): LD_{Lo}: 89 μg/kg
National Technical Information Service, PB83-114298

ETANIDAZOLE

NSC - 301467



Chemical Name:
1*H*-Imidazole-1-acetamide, *N*-(2-hydroxyethyl)-2-nitro-

Other Names:
SR-2508

CAS Registry Number: 22668-01-5

Molecular Formula: $C_7H_{10}N_4O_4$ **M.W.:** 214.2

Approximate Solubility: (mg/mL)

Water	> 100
Methanol	60
Ethanol	30
Chloroform	< 1

Stability:

Bulk:
The sample is stable at room temperature for at least one month (HPLC).

Solution:
As a 10% solution in water, the chemical is stable for at least 24 hours (HPLC).

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max} = 323 ± 2 nm ε = 7,540 - 8,020

High Performance Liquid Chromatography:

Column:	3.9 mm x 30 cm μBondapak C_{18}
Mobile Phase:	100% H_2O
Flow Rate:	1 mL/min
Detection:	UV at 254 nm
Sample Preparation:	1 mg/mL in internal standard solution
Internal Standard:	8.6 mg uracil/100mL H_2O
Retention Volume:	8.6 mL (NSC-301467) 5.6 mL (I.S.)

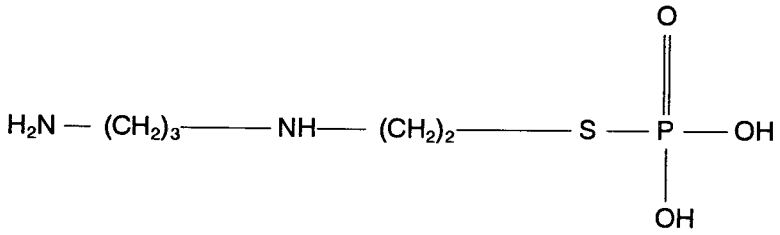
Toxicity Data:

Mouse(ip): LD_{50}: 3300 mg/kg
Radiation Research, 91,186(1982)

Mouse(iv): LD_{50}: 4400 mg/kg
International Journal of Radiation Oncology, Biology and Physics, 12,1097(1986)

ETHIOFOS

NSC - 296961



Chemical Name:
2-[(3-Aminopropyl)amino]ethanethiol, dihydrogen phosphate (ester)

Other Names:
Amifostine (USAN/INN); Gammaphos; WR-2721; Ethyol®

CAS Registry Number: 20537-88-6

Molecular Formula: $C_5H_{15}N_2O_3PS$ **M.W.:** 214.2

Approximate Solubility: (mg/mL)

Water	≈ 450
95% Ethanol	< 0.01
Chloroform	< 0.01
Toluene	< 0.01

Stability:

Bulk:
A small sample stored in a small container at 60 °C showed about 14% decomposition in 24 hours. A small sample stored in a large container at 60 °C for 30 days appeared to be stable. The stability of the compound is dependent on the temperature and the relative amount of moisture present (HPLC and TLC).
The compound should be stored under refrigeration in tightly closed containers.

Solution:
A 5% aqueous solution showed about 1% decomposition after 24 hours at room temperature (TLC).

High Performance Liquid Chromatography:

Column:	C_{18} Reverse Phase, 300 mm x 4 mm i.d.
Mobile Phase:	H_2O
Flow Rate:	1.0 mL/min
Detection:	UV at 200 nm
Sample Preparation:	Immediately prior to injection each sampling was dissolved in 0.10 mL of water
Retention Volume:	4.0 mL (NSC-296961)

Toxicity Data:

Rat(ip): LD_{50}: 418 mg/kg
Radiobiologiya, 16,249,(1976)

Rat(im): LD_{50}: 396 mg/kg
Radiobiologiya, 16,249,(1976)

Mouse(po): LD_{50}: 842 mg/kg
Radiobiologiya, 20,746,(1980)

Mouse(ip): LD_{50}: 321 mg/kg
NCI Screening Program Data Summary

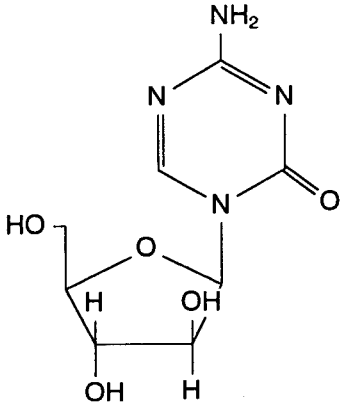
Mouse(iv): LD_{50}: 557 mg/kg
National Technical Information Service, PB81-199580

Mouse (im): LD_{50}: 514 mg/kg
Radiobiologiya, 16,249,(1976)

Dog(iv): LD_{Lo}: 279 mg/kg
Toxicologic Pathology, 13,58,(1985)

FAZARABINE

NSC - 281272



Chemical Name:
4-Amino-1-β-*D*-arabinofuranosyl-1,3,5-triazin-2(1*H*)-one

Other Names:
5-Azacytosine arabinoside; ARA-AC

CAS Registry Number: 65886-71-7

Molecular Formula: $C_8H_{12}N_4O_5$ **M.W.:** 244.2

Approximate Solubility:	(mg/mL)
Water	> 16
Ethanol	insoluble
Dimethylsulfoxide	> 165

Ultraviolet Absorption:

(95% EtOH)

λ_{max} = 243 ± 2 nm ε = 7,150 - 7,350

High Performance Liquid Chromatography:

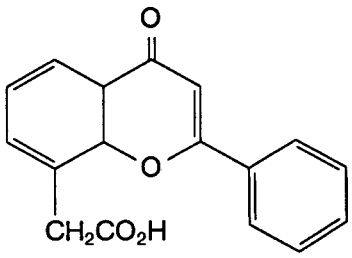
Column:	Waters RCM 100, C_{18}
Mobile Phase:	0.04 M pH 4.6 KH_2PO_4/CH_3OH, 99/1
Flow Rate:	2.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	Methanol solution
Retention Volume:	16.6 mL (NSC-281271)

Optical Rotation:

(c = 1.2, H_2O) $[\alpha]_D^{25}$ = 121.5 ± 2°

FLAVONE ACETIC ACID

NSC - 347512



Chemical Name:
4-Oxo-2-phenyl-4*H*-1-benzopyran-8-acetic acid

Other Names:
Flavone-8-acetic acid

CAS Registry Number: 87626-55-9

Molecular Formula: $C_{17}H_{12}O_4$ **M.W.:** 280.3

Approximate Solubility:	(mg/mL)
Water	< 0.1
0.1 N NaOH	≈ 20
0.1 N HCl	< 0.1
0.1 M $NaHCO_3$	< 0.3
95% EtOH	1
MeOH	1
$CHCl_3$	< 0.1

DMSO	> 100
TFA	> 100
10% DMSO	< 1

Stability:

Bulk:

As a bulk chemical, Flavone-8-acetic acid is stable for at least 3 months at 60 °C (HPLC).

Solution:

Solutions of 1 mg/mL dissolved in 0.1 N NaOH (pH 9) showed no decomposition for at least 27 hours.

High Performance Liquid Chromatography:

Column:	Varian, C_{18}, 5μm, 150 x 4 mm i.d.
Mobile Phase:	MeOH/H_2O/HAc (55/45/0.05)
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	Approximately 0.25 mg/mL is dissolved in internal standard solution
Internal Standard:	m-Nitroaniline (0.15 mg/mL in MeOH)
Retention Volume:	10.4 mL (NSC-347512)

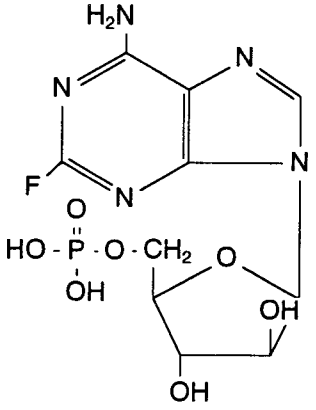
Ultraviolet Absorption:

(95% EtOH)

λ_{max}	ε
296 ± 2nm	21,200 - 21,800
256 ± 2nm	19,000 - 20,300

FLUDARABINE PHOSPHATE

NSC - 312887



Chemical Name:
2-Fluoro-9-(5-*O*-phosphono-β-*D-arabino*-furanosyl)-9*H*-purin-6-amine

Other Names:
2-F-ARA AMP; 2-Fluoroadenine arabinoside-5′-phosphate; Fludara®

CAS Registry Number: 75607-67-9

Molecular Formula: $C_{10}H_{13}FN_5O_7P$ **M.W.:** 365.2

Approximate Solubility: (mg/mL)

Water	9.2
pH 4 buffer	27.6
pH 9 buffer	57

Stability:

Bulk:
Based on HPLC analysis, the sample is stable for at least one month when stored as the bulk chemical at room temperature and 60 °C.

Solution:
A 2 mg/mL aqueous solution is stable for at least 48 hours at room temperature and laboratory illumination (HPLC).

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max} = 262 ± 2 nm ε = 12,600 -13,400

High Performance Liquid Chromatography:

Column:	Alltech ODS, 250 x 4.6 mm i.d.
Mobile Phase:	5% MeOH in 0.1 M KH_2PO_4 buffer, pH 4
Flow Rate:	1.5 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.2 mg/mL in internal standard solution
Internal Standard:	0.3 mg thymidine/mL water
Retention Volume:	13.0 mL (NSC-312887)

19.5 mL (I.S.)

Optical Rotation:

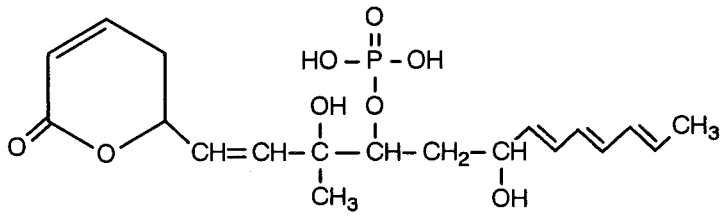
(c = 0.5, H_2O) $[\alpha]_D^{21} = 12 \pm 2°$

Toxicity Data:

Mouse(iv): LD_{50}: 1236 mg/kg
National Technical Information Service, PB83-195685

FOSTRIECIN

NSC - 339638



*Na

Chemical Name: 5,6-Dihydro-6-(3,6,13-trihydroxy-3-methyl-4-(phosphonooxy)-1,7,9,11-tridecatetraenyl)-2*H*-pyran-2-one

Other Names:
Pyranone Phosphate; Antibiotic CI 920; Antibiotic CL 1565A; CI920; CL 1565A;

CAS Registry Number: 87810-56-8

Molecular Formula: $C_{19}H_{26}NaPO_9$ **M.W.:** 452.4

Approximate Solubility:	(mg/mL)
Water	> 300
Methanol	20

Stability:

Bulk:
Decomposition was not observed when the bulk drug was frozen and stored for 23 months in the presence of one molar equivalent of sodium ascorbate.

Solution:
At low concentrations (1.0 mg/mL or less) in the presence of sodium ascorbate, potency is retained upon storage at 5°C for up to three weeks. The compound is most stable in the pH range 4-8, with rapid decomposition occurring in both strongly acidic and strongly basic solutions.

Ultraviolet Absorption:

(Methanol)

λ_{max}	ε
267 ± 2	32,000 - 33,000

High Performance Liquid Chromatography:

Column:	Chemcopak 5-ODS-H, 4.6 x 250 mm i.d.
Mobile Phase:	10% Acetonitrile in pH 7, 0.05M KH_2PO_4
Flow Rate:	1.35 mL/min
Detection:	UV at 254 nm

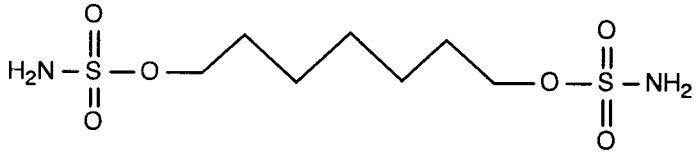
Sample Preparation: In a dry box under nitrogen, samples (≈1.5 mg) are accurately weighed and dissolved in 1.00 mL water. One mL of internal standard is added. 10 μL is injected for analysis.

Internal Standard: ≈40 mg m-nitroaniline in 50 mL of methanol.

Retention Volume: 19.5 mL (NSC 339638)
74.2 mL (I.S.)

HEPSULFAM

NSC - 329680



Chemical Name:
Sulfamic acid, 1,7-heptanediyl ester

CAS Registry Number: 96892-57-8

Molecular Formula: $C_7H_{18}N_2O_6S_2$ **MW.:** 290.4

Approximate Solubility:	(mg/mL)
Water	3.6 - 2.7
Buffer, pH 4	5.0 - 3.3
Buffer, pH 9	5.6 - 3.7
Ethanol	> 10.6
Dimethylacetamide	> 10.0
DMSO	> 11.2

Chloroform	< 0.7
Ethyl acetate	> 9.9
t-Butanol	> 10.0

Stability:

Bulk:
Test samples exposed to room temperature (25 °C) for three months shows very little degradation. Test samples stored at 50 °C in the dark showed significantly greater loss (≈ 10%).

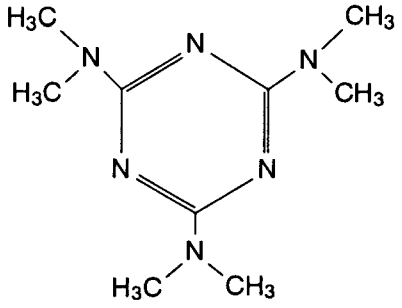
Solution:
A test sample of 25 mg/mL in 30% DMSO/water showed no significant degradation when stored for 48 hr.

High Performance Liquid Chromatography:

Column:	RCM-100, 10 μm C_{18}, 100 x 8 mm (Waters Assoc.)
Mobile Phase:	30% acetonitrile/water (v/v)
Flow Rate:	1.4 mL/min
Detection:	Waters Model R401 Differential Refractometer
Sample Preparation:	≈24 mg/mL in mobile phase
Internal Standard:	≈12.3 mg/mL acetophenone in mobile phase
Retention Volume:	6.1 mL (NSC 329680) 11.8 mL (I.S.)

HEXAMETHYLMELAMINE

NSC - 13875



Chemical Name:
N,N,N′,N′,N″,N″-Hexamethyl-1,3,5-triazine-2,4,6-triamine

Other Names:
HMM; Altretamine (USAN); Hexalen®

CAS Registry Number: 645-05-6

Molecular Formula: $C_9H_{18}N_6$ **M.W.:** 210.3

Approximate Solubility:	(mg/mL)
Water	0.92
Benzene	106
$CHCL_3$	220
EtOAc	52
Et_2O	47

Stability:

Bulk:
The bulk drug is stable at room temperature.

Solution:
Aqueous solutions at pH 4, 7, and 10 are stable for 24 hours at room temperature (UV).

Ultraviolet Absorption:

(Methanol)

λ_{max} = 227 ± 2 nm ε = 51,400 - 52,400

Gas-Liquid Chromatography:

Column: 10% SP-2100 on 80/120 Supelcoport; glass, 1.83 m x 2 mm i.d.

Carrier Gas: Helium

Flow Rate: 30 mL Helium/minute

Temperatures:
Oven 155°C
Isothermal injector 250 °C
Detector 250 °C

Detection: Flame ionization

Internal Standard: Octadecane

Retention Times: 9.6 min (NSC - 13875)
17.8 min (I.S.)

Toxicity Data:

Human(po): TD_{Lo}: 8 mg/kg
Cancer Chemotherapy Reports, 56,505,(1972)

Rat(po): LD_{50}: 350 mg/kg
Principles of Insect Chemosterilization, 315,(1968)

Rat(ip): LD_{50}: 265 mg/kg
Journal of Pharmacology & Experimental Therapeutics, 100,398,50

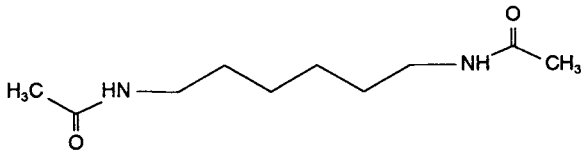
Mouse(po): LD_{50}: 437 mg/kg
Archives Internationales de Pharmacodynamie et de Therapie, 160,83,(1966)

Mouse(ip): LD_{50}: 200 mg/kg
Cancer Research, 40,2762,(1980)

Mouse(iv): LD_{50}: 171 mg/kg
National Technical Information Service, PB293-046

HMBA

NSC - 95580



Chemical Name:
N,N'-Hexamethylenebisacetamide

CAS Registry Number: 3073-59-4

Molecular Formula: $C_{10}H_{20}N_2O_2$ **M.W.:** 200.3

Approximate Solubility:	(mg/mL)
H_2O	> 50
pH 4 Acetate buffer	> 50
pH 9 Carbonate buffer	> 50
0.1 N NaOH	> 50
0.1 N HCL	> 50
10% Ethanol	> 50
95% Ethanol	> 50
Methanol	> 50

Stability:

Bulk:
A sample stored at 60 °C in the dark for 30 days retained 99 ± 2% of its potency (GC).

Solution:
Samples were dissolved in water at a concentration of 20 mg/mL and stored in clear glass containers at room temperatures under normal laboratory light for 9 days. The sample retained 98 ± 2% of its potency (GC).

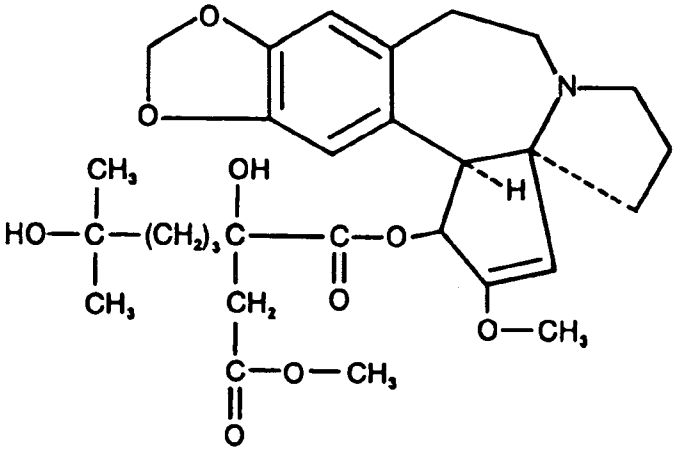
Gas-Liquid Chromatography:

Column:	Packed glass, 10% OV-17 on Gas Chrom Q, 100/120 Mesh, 1.83 m x 2 mm i.d.
Carrier Gas:	Helium
Flow Rate:	30 mL/min
Temperatures:	Oven 205 °C Injector 250 °C Detector 250 °C
Detection:	FID
Retention Times:	6.4 min (NSC - 95580) 10.3 min (I.S.)
Sample Preparation:	1 mg/mL in internal standard solution

Internal Standard:	Pentacosane (0.6 mg/mL in isopropanol/hexane, 70/30)
Retention Times:	6.4 min (NSC-95580) 10.3 min (I.S.)

HOMOHARRINGTONINE

NSC - 141633



Chemical Name: Cephalotaxine, 4-methyl 2-hydroxy-2-(4-hydroxy-4-methylpentyl)butanedioate (ester), [3(*R*)]-

Molecular Formula: $C_{29}H_{39}NO_9$ **M.W.** 545.6

Stability:

Bulk:

Room temperature and 60 °C stability studies indicate the chemical to be stable for at least 30 days (HPLC).

Solution:

Room temperature stability studies for homoharringtonine (1 mg/mL) in 10% ethanol showed 16% decomposition after 24 hours and 35% decomposition after 96 hours (HPLC).

Ultraviolet Absorption:

(Methanol)

λ_{max} **=291 ± 2 nm** ε = 4,000 - 4,250

High Performance Liquid Chromatography:

Column:	Waters RCM C_{18} cartridge
Mobile Phase:	MeOH/water/NH_4OH (75/50/3)
Flow Rate:	3 mL/min
Detection:	UV at 280 nm
Sample Preparation:	1 mg/mL in methanol or internal standard solution
Internal Standard:	strychnine (30 mg/25 mL of MeOH)
Retention Volume:	12.0 mL (NSC-141633) 5.2 mL (I.S.)

Toxicity Data:

Mouse(ip): LD_{50}: 1960 μg/kg
Chinese Medical Journal, 92,175,(1979)

Mouse(ip): LD_{50}: 6.5 mg/kg
Journal of Applied Toxicology,6,270(1986)

HYDRAZINE SULFATE

NSC 150014

$NH_2\text{-}NH_2 \cdot H_2SO_4$

Chemical Name:
Hydrazine, sulfate (1:1)

CAS Registry Number: 10034-93-2

Molecular Formula: $H_6N_2O_4S$ **M.W.:** 130.1

Approximate Solubility: (mg/mL)

Water	≈ .03
Water (hot)	freely soluble
EtOH	insoluble

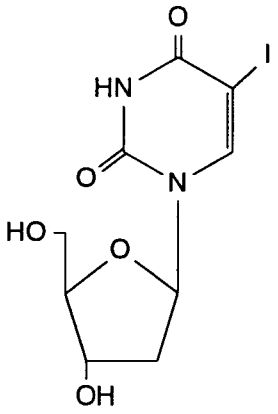
Ion Chromatographic Analysis:

Column:	IC-Pak C (Waters Assoc.) with a Cation Guard Column (Waters Assoc.) installed between the pump and injector.
Injector:	Model 9125 (Rheodyne) with a 20 μL loop or equivalent.
Mobile Phase:	8 mM Nitric Acid/0.05 mM EDTA
Flow Rate:	1.2 mL/min

Detection:	Model 430 Conductivity (Waters Assoc.). 5000 μS range. Polarity negative.
Sample Preparation:	Weighed amounts ($\approx$4 mg) are placed in 50 mL volumetric flasks and diluted to volume with the mobile phase. The diluted samples ($\approx$80 μg/mL) are analyzed directly.
Injection Volume:	20 μL
Temperature:	35 °C (detector only)

IODODEOXYURIDINE

NSC - 39661



Chemical Name:
2′-Deoxy-5-iodouridine

Other Names:
Idoxuridine (USAN); 5-IUdR

CAS Registry Number: 54-42-2

Molecular Formula: $C_9H_{11}IN_2O_5$ **M.W.:** 354.1

Approximate Solubility:	(mg/mL)
0.1 N NaOH	30
0.1 N HCL	2
H_2O	2

Stability:

Bulk:
No changes were found in material stored at room temperature and at 60 °C for 28 days.

Solution:
An aqueous solution (2 mg/mL) shows no decomposition after 24 hours at room temperature (UV and paper chromatography).

Ultraviolet Absorption:

(Water)

λ_{max}= 288 ± 2 nm ε = 7,500 - 7,800

High Performance Liquid Chromatography:

Column:	4.6 mm i.d. x 25 cm Alltech Spherisorb S5 ODS
Mobile Phase:	2% CH_3CN in water
Flow Rate:	2.5 mL/min
Detection:	UV at 254 nm
Sample Preparation:	1 mg/mL in water or internal standard solution
Internal Standard:	adenosine (0.3 mg/mL in 0.01 N NaOH)
Retention Volume:	31 mL (NSC - 39661) 36 mL (I.S.)

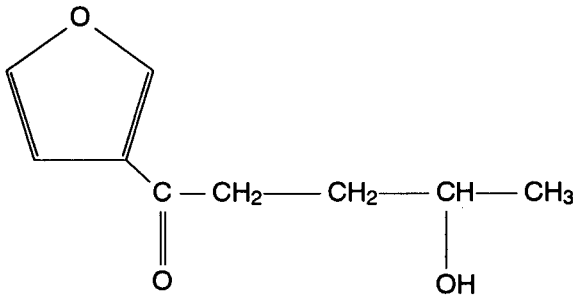
Toxicity Data:

Rat(ip): LD_{50}: 4000 mg/kg
Advances in Teratology, 3,181,(1968)

Mouse(ip): LD_{50}: 1000 mg/kg
Journal of the National Cancer Institute, 62,911,(1979)

IPOMEANOL

NSC - 349438



Chemical Name:
1-(3-Furanyl)-4-hydroxy-1-pentanone

CAS Registry Number: 55659-41-1

Molecular Formula: $C_9H_{12}O_3$ **M.W.:** 168.2

Approximate Solubility: (mg/mL)

Chloroform	> 100
Methanol	> 100
Water	≈ 20
10% propylene glycol, 10% EtOH in water	≈ 20
0.1 N HCl	≈ 55
0.1 N NaOH	< 3

Stability:

Bulk:
4-Ipomeanol is stable when stored at freezer temperatures (-18°C)

Solution:
Aqueous solutions are stable for at least 24 hr over a pH range of 3 to 8.

Ultraviolet Absorption:

(100% EtOH)

λ_{max} = 250 ± 2 nm ε = 3340 ± 200

High Performance Liquid Chromatography:

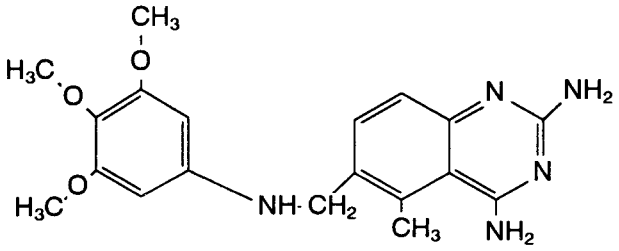
Column:	IBM C_{18}, 250 mm x 4.5 mm i.d.
Mobile Phase:	30% methanol in water
Flow Rate:	1 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.7 mg/mL in mobile phase
Internal Standard:	*m*-nitrophenol (7 mg dissolved in 10 mL MeOH)
Retention Volume:	12.7 mL (NSC 349438) 22.9 mL (I.S.)

Optical Rotation:

(c = 1.1,CCl_4) $[\alpha]_D^{20}$ = 1.0 ± 0.2°

JB-11

NSC - 249008



*CH_3COOH

Chemical Name:
5-Methyl-6-[[(3,4,5-trimethoxyphenyl)amino]methyl]-2,4-quinazolinediamine, acetate

CAS Registry Number: 52128-35-5

Molecular Formula: $C_{19}H_{23}N_5O_3 \cdot CH_3COOH$ **M.W.:**429.5

Approximate Solubility: (mg/mL)

Water	1 - 2
pH 4 Acetate buffer	< 1
pH 9 Acetate buffer	< 1
0.1 N HCl	1 - 5
0.1 N NaOH	< 1
Methanol	12 - 15
95% Ethanol	1 - 5
10% Ethanol	1 - 3
Dimethylacetamide	10 - 15
Dimethylsulfoxide	≈100

Stability:

Bulk:
A sample stored at 60 °C for 30 days showed no decomposition (UV, HPLC).

Solution:
A solution in 5% methanol (0.5 mg/mL) showed no decomposition after 9 days (UV). A solution in 5% dimethylacetamide/pH 4 acetate buffer showed no decomposition after 48 hours(HPLC).

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{max}	ε
237 ± 2 nm	46,970 - 47,922
341 ± 2 nm	4,410 - 4,680

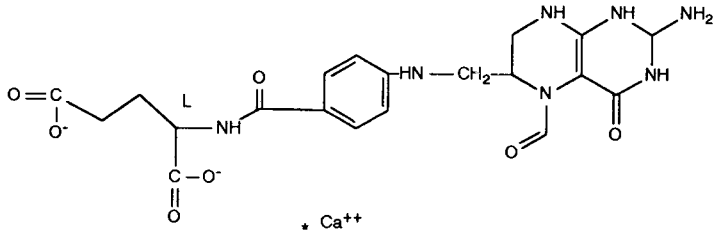
High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 300 x 3.9 mm i.d.
Mobile Phase:	CH_3CN/3% acetic acid in water, 20/80, v/v
Flow Rate:	0.8 mL/min
Detection:	UV at 254 nm

Sample Preparation:	0.5 mg/mL in methanol containing internal standard
Internal Standard:	0.35 mL/mL acetophenone in methanol
Retention Volume:	6.4 mL (NSC-249008) 9.1 mL (I.S.)

LEUCOVORIN CALCIUM

NSC - 3590



Chemical Name:
N-[4-[[(2-Amino-5-formyl-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-*L*-glutamic acid, calcium salt (1:1), (*R,S*)-

Other Names:
Citrovorum Factor; Folinic Acid; Calcium Leucovorin

CAS Registry Number: 1492-18-8

Molecular Formula: $C_{20}H_{23}CaN_7O_7$ **M.W.:** 511.5

Approximate Solubility: (mg/mL)

DMSO	<< 1
H_2O	100
0.1 N NaOH	< 20

Stability:

Bulk:
Calcium leucovorin was stable in bulk form after 4 weeks storage at 60 °C (HPLC).

Solution:
Leucovorin in 0.1 N NaOH (pH 13) and in deionized water (pH 6) was stable at room temperature under laboratory illumination for at least 24 hours (HPLC).

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{max} = 282 ± 2 nm ε = 23,000 - 26,500

High Performance Liquid Chromatography:

Column:	30 cm x 4 mm i.d. Spherisorb ODS
Mobile Phase:	15% MeOH in 0.1 M KH_2PO_4, pH adjusted to 4.0
Flow Rate:	1.5 mL/min
Detection:	UV at 254 nm
Sample Preparation:	1 mg/mL in water or internal standard solution
Internal Standard:	Folic acid (1 mg/mL in 0.02 N NaOH)
Retention Volume:	12.0 mL (NSC -3590) 20.2 mL (I.S.)

Optical Rotation:

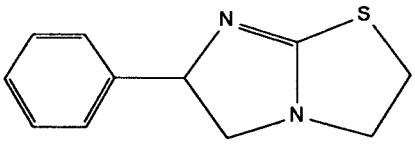
(c = 1, H_2O) $[\alpha]_D^{20} = 13.0 \pm 2°$

Toxicity Data:

Mouse(iv): LD_{50}: 732 mg/kg
Drugs in Japan. Ethical Drugs. 6,910,(1982)

LEVAMISOLE

NSC - 177023



*HCl

Chemical Name:
2,3,5,6-Tetrahydro-6-phenylimidazo[2,1-*b*]thiazole, (*S*)-, hydrochloride

Other Names:
Tetramisole; Tetramizole

CAS Registry Number: 16595-80-5

Molecular Formula: $C_{11}H_{12}N_2S \cdot HCl$ **M.W.:**241.0

Approximate Solubility: (mg/mL)

Water	210
Methanol	sol.
Propylene glycol	sol.
Ethanol	sl. sol.

Stability:

Bulk:
Levamisole appears to be stable in the bulk form at 60 °C for at least four weeks.

Solution:
At 100 mg/mL concentrations in water and pH 7 buffer, the compound is stable for at least 9 days when stored at ambient temperature under normal laboratory illumination.

Ultraviolet Absorption:

(0.1N HCl)

λ_{max}	ε
213 ± 2 nm	20100 ± 200

High Performance Liquid Chromatography:

Column:	IBM C_8, 150 x 4 mm i.d., 5µm, end capped
Mobile Phase:	Methanol/0.1 M, pH 7, KH_2PO_4 (1/1)
Flow Rate:	1.5 mL/min
Detection:	254 nm

Sample Preparation: ≈0.5 mg is accurately weighed and then dissolved in 1.00 mL of water with the aid of brief sonication, interspersed with vigorous mixing. 0.05 mL of the internal solution is then added and mixed.

Internal Standard: 1.7 mg of *m*-nitroaniline in 25 mL of methanol

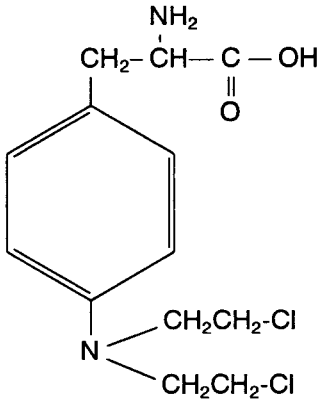
Retention Volume: 11.2 mL (NSC 177023)
4.5 mL (I.S.)

Optical Rotation:

(c = 1, H_2O) $[\alpha]_D^{21}$ = -126.2 ± 1.4°

MELPHALAN

NSC - 8806



Chemical Name: 4-[Bis(2-chloroethyl)amino-*L*-phenylalanine

Other Names: *L*-PAM; *L*-sarcolysine; Alkeran®; Sarcoclorin

CAS Registry Number: 3223-07-2

Molecular Formula: $C_{13}H_{18}Cl_2N_2O_2$ **M.W.=** 305.2

Approximate Solubility:	(mg/mL)
95% ethanol	<0.9
10% aqueous ethanol	≈1.3
Methanol	2.8 - 5.6
Water	1.7 - 2.3
Chloroform	<1
0.1 N HCL	9 - 17
0.1 N NaOH	7 - 10.6
Acetone	<1

pH 4 citrate buffer	2.2 - 2.6
pH 9 borate buffer	2.0 - 2.4

Stability:

Bulk:
A dried sample, stored at 60 °C for 15 days, showed about 10% decomposition as indicated by UV absorption and ionic chloride content.

Solution:
After 24 hours in water at 28°C, approximately 80% decomposition was observed (TLC).

Ultraviolet Absorption:

(H_2O)

λ_{max} = 260 ± 2 nm ε = 17,410 - 17,880

High Performance Liquid Chromatography:

Column:	Beckman Ultrasphere, 5μ, 250 x 4.6 mm i.d.
Mobile Phase:	Methanol: 10 mM phosphate buffer, adjusted to pH 3.0 with phosphoric acid
Flow Rate:	1 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.2 mg/mL in methanol

Internal Standard: Propriophenone, 0.2 μL/mL

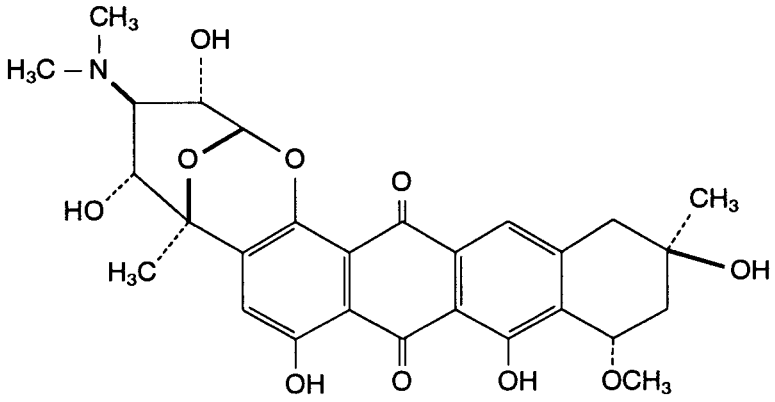
Retention Volume: 11.8 mL (NSC - 8806)
15.9 mL (I.S.)

Optical Rotation:

(c = 0.7, methanol on a dried basis) $[\alpha]_D^{24} = -31.5 \pm 2°$

MENOGARIL

NSC - 269148



Chemical Name:4-(Dimethylamino)-3,4,5,6,11,12,13,14-octahydro-3,5,8,10,13-pentahydroxy-11-methoxy-6,13-dimethyl-2,6-epoxy-2*H*-naphthaceno[1,2-*b*]-oxocin-9,16-dione, (*2*α,*3*β,*4*α,*5*β,*6*α,*11*α,*13*α)-, (*P*)-

Other Names:
7-con-O-Methylnogarol; 7-OMEN

CAS Registry Number: 71628-96-1

Molecular Formula: $C_{28}H_{31}NO_{10}$ **M.W.:** 541.6

Approximate Solubility: (mg/mL)

H_2O	insoluble (<0.01)
pH 5, 0.1 M Phosphate buffer	insoluble (<0.01)
pH 9, 0.1 M Phosphate buffer	insoluble (<0.01)
95% EtOH	0.05
10% aq. DMA	0.8

DSMO	4
DMA	10

Stability:

Bulk:
Bulk stability studies indicate slight, gradual decomposition occurring over 30 days at room temperature and laboratory illumination; total decomposition was approximated at 2%. Stored at 60 °C and in darkness, the sample is stable for at least 30 days (HPLC and TLC).

Solution:

Menogaril solutions (0.1 and 5 mg/mL are stable for at least 14 days at room temperature in the dark.

Ultraviolet Absorption:

(95% EtOH)

λ_{max}	ε
478 ± 2 nm	15,000 - 15,200
259 ± 2 nm	23,000 - 24,000
235 ± 2 nm	48,400 - 49,800

High Performance Liquid Chromatography:

Column:	Zorbax TMS, 250 mm x 4.6 mm i.d.
Mobile Phase:	0.1 M KH_2PO_4, pH 5.6/CH_3OH, 45/55
Flow Rate:	1.0 mL/min

Detection: UV at 254 nm

Retention Volume: 7.1 mL (NSC-269148)

Optical Rotation:

(c = 0.15, $CHCl_3$) $[\alpha]_D^{21} = 920 \pm 13°$

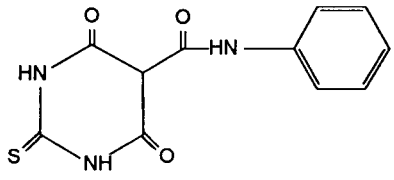
Toxicity Data:

Rat(iv): LD_{50}: 77400 μg/kg
National Technical Information Services, PB84-148410

Mouse(ip): LD_{50}: 83500 μg/kg
National Technical Information Services, PB84-148410

MERBARONE

NSC - 336628



Chemical Name:
Hexahydro-4,6-dioxo-*N*-phenyl-2-thioxo-5-pyridinecarboxamide

Other Names:
5-Carboxyanilino-2-thiobarbituric acid

CAS Registry Number: 97534-21-9

Molecular Formula: $C_{11}H_9N_3O_3S$ **M.W.:** 263.3

Approximate Solubility:	(mg/mL)
H_2O	< 0.1
C_2H_5OH	< 0.1
0.1N HCl	< 0.1
DMSO	80
0.1N NaOH	5
$CHCl_3$	< 0.1
CH_3CN	< 0.1
pH 9 buffer	< 0.1
$(CH_3)_2CO$	< 0.1

TFA	< 0.1
THF	6

Stability:

Bulk:
As a bulk chemical, Merbarone is found to be stable at 25 and 45 °C for at least 4 weeks (HPLC).

Solution:
As a 1 mg/mL pH 9 buffered solution at room temperature (25 ± 2 °C), Merbarone appeared stable for at least 24 hours (HPLC).

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{max}	ε
306 ± 2 nm	29,600 - 30,300
243 ± 2 nm	17,000 - 17,500

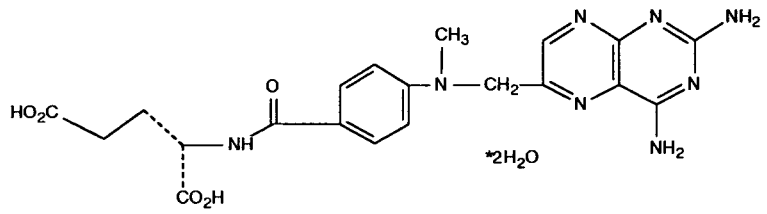
High Performance Liquid Chromatography:

Column:	Hamilton PRP-1, 250 x 4.1 mm i.d.
Mobile Phase:	14% CH_3CN in 0.1 M Na_2HPO_4 (pH adjusted to 10.2 with NaOH)
Flow Rate:	1.5 mL/min

Detection:	UV at 243 nm
Sample Preparation:	Approximately 1 mg of sample dissolved in 2 mL of mobile phase plus one drop of 5N NaOH
Retention Volume:	7.3 mL (NSC-336628)

METHOTREXATE

NSC - 740



Chemical Name: *N*-[4-[[(2,4-diamino-6-pteridinyl)-methyl]methylamino]benzoyl]glutamic acid, dihydrate

Other Names:
MTX; Amethopterine; 4-amino-10-methylfolic acid

CAS Registry Number: 59-05-2

Molecular Formula: $C_{20}H_{22}N_8O_5.2H_2O$ **M.W.:**490.5

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{max}	ε
258 ± 2 nm	22,800 - 25,200
303 ± 2 nm	23,200 - 25,200
372 ± 2 nm	7,350 - 8,200

High Performance Liquid Chromatography:

Column:	300 mm x 4 mm i.d. Spherisorb ODS
Mobile Phase:	20% CH_3OH in 0.1 M KH_2PO_4 at pH 6.7
Flow Rate:	2 mL/min
Detection:	UV at 254 nm
Sample Preparation:	1 mg sample in 1.0 mL 0.02 N NaOH or internal standard solution
Internal Standard:	5 mg 4-deoxy-4-amino-N^{10}-methylpteroic acid/5 mL 0.02 N NaOH
Retention Volume:	11.5 mL (NSC 740) 19.0 mL (I.S.)

Optical Rotation:

(c = 1, 0.05 M Na_2CO_3) $[\alpha]_D^{20}$ = +17.0 - 19.5°

Toxicity Data:

Man(iv): TD_{Lo}: 740 mg/kg
Archives of Internal Medicine,136,1321(1976)

Mouse(ip): LD_{50}: 50 mg/kg
Anatomical Record 178,465(1974)

Rat(po): LD_{50}: 135 mg/kg
Drugs in Japan. Ethical Drugs, 6th Ed.,(1982),p841

Rat(ip): LD_{50}: 6 mg/kg
Drugs in Japan. Ethical Drugs, 6th Ed.,(1982),p841

N-METHYLFORMAMIDE

NSC - 3051

CH_3-NHCH(=O)

Chemical Name: *N*-Methylformamide

Other Name: NMF

CAS Registry Number: 123-39-7

Molecular Formula: C_2H_5NO **M.W.:** 59.1

Approximate Solubility:

Water	miscible
Ethanol	miscible
Ether	immiscible

Stability:

Solution:
A 25% aqueous solution is stable at room temperature for at least one week (NMR).

Ultraviolet Absorption:

(H_2O)

The spectrum shows an end absorption with a small shoulder at 280 nm.

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 3.9 mm i.d. x 30 cm
Mobile Phase:	3% CH_3CN
Flow Rate:	1 mL/min
Detection:	UV at 220 nm
Sample Preparation:	8 mg/mL in mobile phase or internal standard solution
Internal Standard:	dimethylacetamide (2mg/mL in mobile phase)
Retention Volume:	4.5 mL (NSC - 3051) 9.0 mL (I.S.)

Toxicity Data:

Rat(po): LD_{50}: 4000 mg/kg
Journal of Reproduction and Fertility, 4,219,(1962)

Rat(po): LD_{50}: 3500 mg/kg
Journal of Reproduction and Fertility, 4,219,(1962)

Mouse(po): LD_{50}: 2600 mg/kg
Toxicology (Elsevier), 34,173,(1985)

Mouse(ip): LD_{50}: 2300 mg/kg
Toxicology (Elsevier), 34,173,(1985)

Mouse(sc): LD_{50}: 3100 mg/kg
Dissertation Abstracts International, 40,549,(1979)

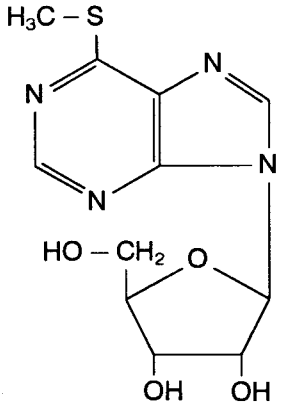
Mouse(iv): LD_{50}: 1580 mg/kg
Toxicology (Elsevier), 34,173,(1985)

Mouse(im): LD_{50}: 2700 mg/kg
Toxicology (Elsevier), 34,173,(1985)

Dog(iv): LD_{10}: 1262 mg/kg
National Technical Information Service, PB82-232158

6-METHYLMERCAPTOPURINE RIBOSIDE

NSC - 40774



Chemical Name:
6-Methylthio-9-β-*D*-ribofuranosyl-9*H*-purine

Other Names:
6-MMPR; 6-Methyl MP-riboside; 6-Methyl-mercaptopurine riboside

CAS Registry Number: 342-69-8

Molecular Formula: $C_{11}H_{14}N_4O_4S$ **M.W.:** 298.3

Approximate Solubility: (mg/mL)

DMA	167
50% DMF	50
H_2O	25
Propylene glycol	6

Stability:

Bulk:
The compound is stable to light and air, mildly decomposed by heat and acid, and is totally degraded by base and peroxidant (HPLC).

Solution:
A saturated solution at room temperature showed no detectable decomposition after 10 days (paper chromatography).

Ultraviolet Absorption:

(Water)

λ_{max}	ε
292 ± 2 nm	19,000 - 19,600
224 ± 2 nm	11,500 - 12,200

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 300 mm x 3.9 mm i.d.
Mobile Phase:	Acetonitrile/water, 12/88, v/v
Flow Rate:	1 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.2 mg/mL in water or internal standard solution

Internal Standard: acetanilide (0.05 mg/mL in water)

Retention Volume: 13 mL (NSC - 40774)
20 mL (I.S.)

Optical Rotation:

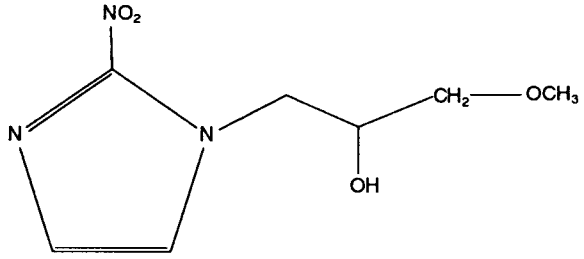
(c = 1, H_2O) $[\alpha]_D^{22} = -58.0 \pm 2°$

Toxicity Data:

Rat(ip): LD_{50}: 65 mg/kg
Archives of Pathology, 86,395,(1968)

MISONIDAZOLE

NSC - 261037



Chemical Name:
α-(Methoxymethyl)-2-nitro-1*H*-imidazole-1-ethanol

Other Names:
Ro-7-0582; 1-(2-Nitroimidazolyl)-3-methoxy-2-propanol;

CAS Registry Number: 13551-87-6

Molecular Formula: $C_7H_{11}N_3O_4$ **M.W.:** 201.2

Approximate Solubility: (mg/mL)

Water	8
Methanol	70
Ethanol	10
Chloroform	10
Acetone	50
Ethyl acetate	8
Dimethylsulfoxide	> 100
Trifluoroethanol	> 100

Stability:

Bulk:
Protected from light, a sample stored for 90 days at 60 °C showed no decomposition (UV or TLC). Exposed to light, a sample at room temperature showed 3% decomposition after 90 days.

Solution:
A solution in 0.1 N HCl showed no decomposition after 4 days. As a 2% solution at room temperature with and without light, the compound is also stable for at least 4 days. When kept in the refrigerator for 15 days <1% decomposition occurs (TLC).

Ultraviolet Absorption:

(95% EtOH)

λ_{max} = 316 ± 2 nm ε = 7,060 - 7,400

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 3.9 mm x 30 cm
Mobile Phase:	30% MeOH in H_2O
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Retention Volume:	6.0 mL (NSC-261037)

Toxicity Data:

Rat(po): LD_{50}: 2131 mg/kg
National Technical Information Service, PB81-121212

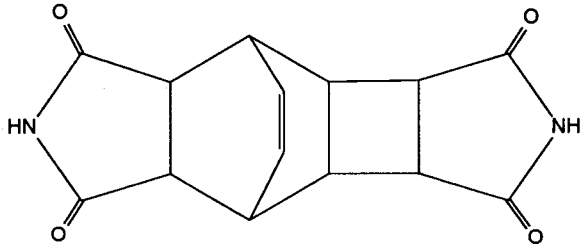
Mouse(po): LD_{50}: 1869 mg/kg
NCI Screening Program Data Summary

Mouse(ip): LD_{50}: 1340 mg/kg
Radiation Research, 91,816,(1982)

Mouse(sc): LD_{50}: 1414 mg/kg
Antimicrobial Agents and Chemotherapy, 513,(1967)

MITINDOMIDE

NSC - 284356



Chemical Name:
Octahydro-4,8-ethenopyrrolo[3′,4′:3,4]cyclobut[1,2-*f*]isoindole-1,3,5,7-(2*H*,6*H*)-tetrone

CAS Registry Number: 10403-51-7

Molecular Formula: $C_{14}H_{12}N_2O_4$ **M.W.:** 272.3

Approximate Solubility: (mg/mL)

p-dioxane	slightly soluble
Aqueous NaOH (2 moles NaOH per mole of compound)	> 20

Stability:

Solution:
A solution was prepared by dissolving 100 mg of drug in 3.0 mL of 0.25 N NaOH. This solution was diluted to 5.0 mL with water to give a final concentration of 20 mg/mL. At room temperature this solution shows 10% decomposition in 40 minutes and 50% decomposition in 5 hours (HPLC).

Ultraviolet Absorption:

(p-dioxane)

λ_{max} = 252 ± 2 nm ε = 346 - 366

High Performance Liquid Chromatography:

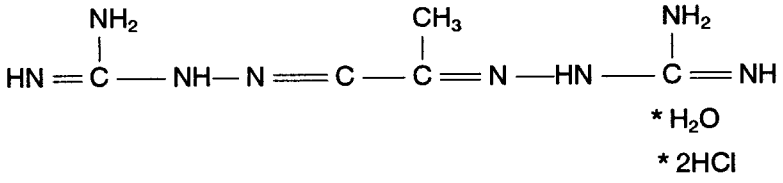
Column:	300 mm x 4.6 mm i.d. RP-8
Mobile Phase:	10% CH_3CN in H_2O, pH adjusted to 4 with acetic acid
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	A 3.4-mg sampling is quickly dissolved in 1.0 mL of 0.05 N NaOH with the aid of sonication and vigorous mixing. At exactly 1.0 min after addition of the solvent the solution is chromatographed.
Retention Volume:	8.1 mL (NSC-284356)

Toxicity Data:

Mouse(iv): LD_{50}: 193 mg/kg
NCI Screening Program Data Summary

MITOGUAZONE

NSC - 32946



Chemical Name:
2,2′-(1-Methyl-1,2-ethanediylidene)bis(hydrazinecarboximidamide), dihdrochloride, monohydrate

Other Names:
Methyl GAG; Methylglyoxal Bisguanylhydrazone Dihydrochloride

CAS Registry Number: 7059-23-6

Molecular Formula: $C_5H_{12}N_8 \cdot 2HCl \cdot H_2O$ **M.W:** 275.1

Approximate Solubility:	(mg/mL)
0.1 N NaOH	soluble
Water	> 100
0.01 N NaOH	partly soluble
0.1 N HCl	partly soluble
MeOH	partly soluble
50% EtOH	partly soluble

Stability:

Solution:
A solution of 100 mg/mL in water stored at room temperature for 44 days showed no decomposition.

Ultraviolet Absorption:

(0.1 N HCl)

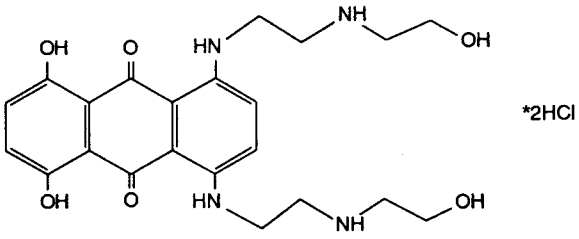
λ_{max} = 283 ± 2 nm ε = 36,200 - 40,000

High Performance Liquid Chromatography:

Column:	4 mm i.d. x 300 mm Spherisorb ODS
Mobile Phase:	4% acetonitrile in 0.1 M KH_2PO_4, pH adjusted to 3.8 with H_3PO_4
Flow Rate:	2 mL/min
Detection:	UV at 210 nm
Sample Preparation:	1 mg/mL in water or internal standard solution
Internal Standard:	1-naphthol-4-sulfonic acid Na salt (7 mg in 25 mL water)
Retention Volumes:	8.0 mL (NSC - 32946) 11.0 mL (I.S.)

MITOXANTRONE HYDROCHLORIDE

NSC - 301739



Chemical Name:
1,4-Dihydroxy-5,8-bis[[2-[(2-hydroxyethyl)amino]ethyl]amino]-9,10-anthracenedione, dihydrochloride

Other Names:
CL 232,315; DHAQ; DHAD; Dihydroxyanthracenedione dihydrochloride

CAS Registry Number: 70476-82-3

Molecular Formula: $C_{22}H_{28}N_4O_6 \cdot 2HCl$ **M.W.:** 517.4

Approximate Solubility:	(mg/mL)
H_2O	5 - 10
pH 4 Acetate buffer	3 - 5
pH 9 Borate buffer	< 1
0.1 N HCl	1 - 3
0.1 N NaOH	decomposes
10% Ethanol	3 - 5
95% Ethanol	< 1
Methanol	< 1

Stability:

Bulk:
After 30 days at 60 °C, no decomposition was observed (UV or TLC).

Solution:
The solution undergoes 6% decomposition in H_2O over 5 days (UV).

Ultraviolet Absorption:

(Methanol)

λ_{max}	ε
670 ± 2 nm	25,230 - 25,270
617 ± 2 nm	19,850 - 19,930
277 ± 2 nm	13,360 - 13,400
241 ± 2 nm	40,000 - 40,920

High Performance Liquid Chromatography:

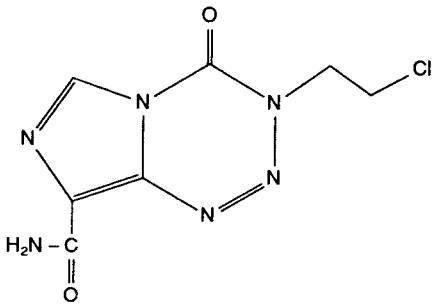
Column:	μPhenyl Porasil, 300 x 4 mm i.d.
Mobile Phase:	CH_3OH/1.5% acetic acid in H_2O with 0.005 M heptanesulfonic acid, 50/50, v/v
Flow Rate:	1.5 mL/min
Detection:	UV at 254 nm
Sample Preparation:	Sample solvent - CH_3OH/pH 4 acetate buffer, 25/75, v/v

Internal Standard: Hexaphenone 15 μL/L sample solvent

Retention Volume: 16.5 mL (NSC-301739)
36 mL (I.S.)

MITOZOLOMIDE

NSC - 353451



Chemical Name:
3-(2-Chloroethyl)-3,4-dihydro-4-oxoimidazo[5,1,-*d*]-1,2,3,5-tetrazine-8-carboxamide

Other Names: Azolastone

CAS Registry Number: 85622-95-3

Molecular Formula: $C_7H_7ClN_6O_2$ **M.W.:** 242.5

Approximate Solubility:	(mg/mL)
H_2O	0.0
Buffer, pH 4	0.0
Buffer, pH 9	≤ 0.7
EtOH	0.0
DMA	≤ 4.9
DMSO	≤ 5.1
$CHCl_3$	≤ 0.7
EtOAc	0.0
t-BuOH	0.0
90% BuOH	≤ 0.8

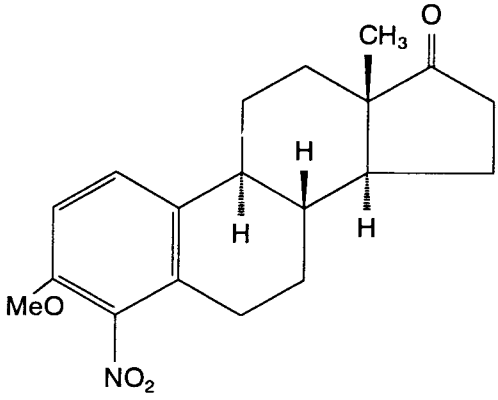
Ether	0.0
THF	≤ 2.0

High Performance Liquid Chromatography:

Column:	RCM-100, 10 μm C_{18}, 100 x 8 mm i.d.
Mobile Phase:	10% CH_3CN/water containing 0.005M sodium heptanesulfonate, pH adjusted to 3 with acetic acid.
Flow Rate:	2.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	8.0 mg sample diluted to 5 mL with internal standard solution.
Internal Standard:	3-(2-hydroxyethyl)-1,2,3-benzotriazinone (2.0 mg/mL in DMSO).
Retention Volume:	13.7 mL (NSC-353451) 20.5 mL (I.S.)

4-NITROESTRONE

NSC - 321803



Chemical Name:
3-Methoxy-4-nitroestra-1,3,5[10]-trien-17-one

Other Names:
4-Nitroestrone, methyl ether

CAS Registry Number: 14846-62-9

Molecular Formula: $C_{19}H_{23}NO_4$ **M.W.:** 329.4

Approximate Solubility:	(mg/mL)
H_2O	< 0.66
Buffer, pH 4	< 0.65
Buffer, pH 9	< 0.65
Ethanol	0.69 - 0.73
DMA	≥ 11.60
DMSO	4.27 - 6.41
$CHCl_3$	≥ 11.60

Ethyl Acetate	4.60 - 9.20
t-Butanol	< 0.65
THF	5.16 - 10.30
CH_3CN	5.02 - 10.00
$DMSO/H_2O$ (60%)	< 0.66
DMA/H_2O (10%)	< 0.66
$EtOH/H_2O$ (10%)	< 0.66

Stability:

Bulk:
A sample stored at 50 °C for 3 months showed no decomposition (HPLC).

Solution:
A 0.06 mg/mL solution of drug in 60% $DMSO/H_2O$ at room temperature showed 10% drug decomposition in 5.41 hours (HPLC).

Ultraviolet Absorption:

(Acetonitrile)

λ_{max}	ε
254 ± 2 nm	1,100 - 1,400
275 ± 2 nm	1,577 - 1,700

High Performance Liquid Chromatography:

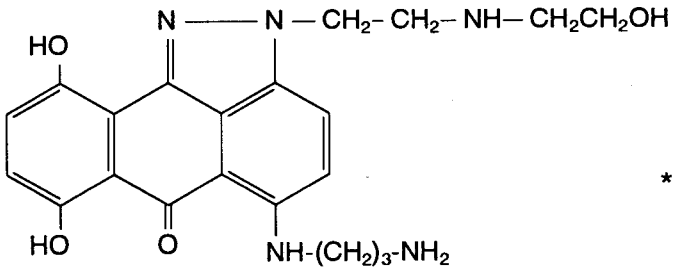
Column: μBondapak C_{18}, 300 x 3.9 nm i.d.

Mobile Phase: 55% CH_3CN in H_2O

Flow Rate:	2 mL/min
Detection:	UV at 254 nm
Sample Preparation:	4.0 mg/mL of sample, 0.32 mg/mL internal standard in dimethylacetamide
Internal Standard:	Norgestrel
Retention Volume:	23.0 mL (NSC-321803) 11.1 mL (I.S.)

PIROXANTRONE

NSC - 349174



Chemical Name:
Anthra[1,9-*cd*]pyrazol-6(2*H*)-one, 5-[3-(aminopropyl)amino]-7,10-dihydroxy-2-[2-[(2-hydroxyethyl)amino]ethyl]-, dihydrochloride

Other Names:
Anthrapyrazole derivative; Oxantrazole

CAS Registry Number: 105118-12-5

Molecular Formula: $C_{21}H_{25}N_5O_4 \cdot 2HCl$ **M.W.:** 484.4

Approximate Solubility:	(mg/mL)
H_2O	> 11.20
Buffer, pH4	> 9.60
Buffer, pH9	> 11.50
Ethanol	< 0.73

DMA	0.70
DMSO	> 9.60
$CHCl_3$	< 0.77
EtOAc	< 0.71
t-BuOH	< 0.71

Stability:

Bulk:
Samples stored at 25 °C under both light and dark conditions at 50 °C in the dark for three months showed no significant degradation (HPLC).

Solution:
A solution containing 10.2 mg/mL in water showed approximately 5% degradation in 24 hours. The test sample exhibited < 10% degradation in 48 hours.

Ultraviolet Absorption:

(H_2O)

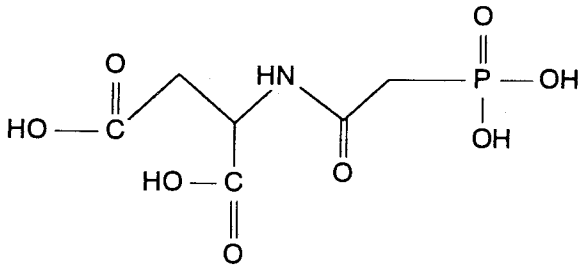
λ_{max}	ε
254 ± 2nm	10,358 ± 500
295 ± 2nm	6,146 ± 400
318 ± 2nm	6,889 ± 400
333 ± 2nm	6,677 ± 400
406 ± 2nm	4,827 ± 400
515 ± 2nm	16,592 ± 600

High Performance Liquid Chromatography:

Column:	Zorbax C_8, 250 x 4.6 mm i.d., 30 x 4.6 mm i.d.
Mobile Phase:	5% CH_3CN/20% DMF /75% (0.2M ammonium acetate/L mobile phase, adjusted with acetic acid to pH 4.5.)
Flow Rate:	1 mL/min
Detection:	UV at 254 nm
Sample Preparation:	10 mg of sample diluted to 10 mL with internal standard solution.
Internal Standard:	1.0 mg/mL benzamide in water
Retention Volume:	11.14 mL (NSC-349174) 6.17 mL (I.S.)

PALA

NSC - 224131



Chemical Name:
N-(Phosphonoacetyl)-*L*-aspartic acid, disodium salt

Other Names:
N-Phosphonoacetyl-*L*-Aspartate Disodium; Sparfosate Sodium (USAN)

CAS Registry Number: 60342-56-5

Molecular Formula: $C_6H_8NO_8P \cdot 2Na$ **M.W.:** 299.1

Approximate Solubility:	(mg/mL)
Water	> 950

Stability:

Bulk:
The compound is very stable as the bulk drug. The bulk material is hygroscopic; protect from moisture when storing.

Solution:
The compound is very stable in aqueous solution (qualitative). PALA (1mg/mL) is chemically stable for at least 2 weeks at room temperature in aqueous solution.

High Performance Liquid Chromatography:

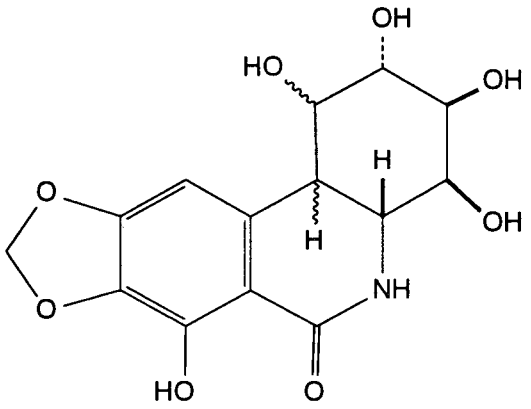
Column:	Partisil PXS 10/25 SAX, 250 mm x 4.6 mm i.d.
Mobile Phase:	0.30 M KH_2PO_4, adjusted to pH 4.0 with H_3PO_4
Flow Rate:	2.0 mL/min
Detection:	UV at 210 nm
Sample Preparation:	2 mg/mL in water or internal standard solution
Internal Standard:	1-naphthol-4-sulfonic acid, Na salt (2 mg/50mL of water)
Retention Volume:	10.8 mL (NSC-224131)

Optical Rotation:

(c = 1, H_2O) $[\alpha]_D^{20} = +14.2 \pm 2°$

PANCRATISTATIN

NSC - 349156



Chemical Name:
1,3,4,4a,5,11b-Hexahydro-1,2,3,4,7-pentahydroxy(1,3)dioxolo-(4,5-*j*)phenanthridin-6(2*H*)-one, (*1R-(1*α,*2*β,*3*α, *4*α,*4a*α,*11b*β))-

CAS Registry Number: 96203-70-2

Molecular Formula: $C_{14}H_{15}NO_8$ **M.W.:** 325.3

Approximate Solubility:	(mg/mL)
H_2O	< 1
Acetate buffer (pH4)	< 1
Carbonate buffer (pH9)	< 1
0.1 N HCl	< 1
0.1 N NaOH	≈ 5-7
MeOH	< 1
95% EtOH	< 1
10% EtOH	< 1

$CHCl_3$	< 1
DMF	10-15

Stability:

Bulk:
The bulk drug was determined to be stable at 60 °C under both light and dark conditions for 30 days (HPLC).

Solution:
Pancratistatin was stable in 50% DMSO/H_2O for 24 hours (HPLC).

Ultraviolet Absorption:

(0.1N NaOH)

λ_{max}	ε
332 ± 2nm	4,000 - 4,100
280 ± 2nm	5,700 - 6,000
233 ± 2nm	23,800 - 24,800

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 10μ, 300 x 3.9 mm i.d.
Mobile Phase:	CH_3CN/10 mM HOAc (10/907, v/v)
Flow Rate:	1.0 mL/min
Detection:	UV at 280 nm

Sample preparation: Sample is dissolved in DMSO to give a concentration of ≈0.65 mg/mL. Internal standard concentration is 0.2 mg/mL.

Internal Standard: Theophylline (1.035 mg/mL in DMSO).

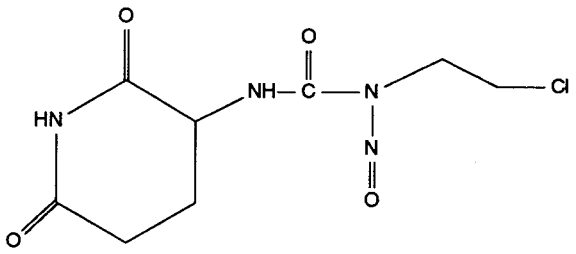
Retention Volume: 18.3 mL (NSC-349156)
8.6 mL (I.S.)

Optical Rotation:

(c = 1, H_2O) $[\alpha]_D^{25} = +44 \pm 2°$

PCNU

NSC - 95466



Chemical Name: *N*-(2-Chloroethyl)-*N'*-(2,6-dioxo-3-piperidinyl)-*N*-nitrosourea

CAS Registry Number: 13909-02-9

Molecular Formula: $C_8H_{11}ClN_4O_4$ **M.W.:** 262.7

Approximate Solubility:	(mg/mL)
Water	< 1
Water pH 4	< 1
Water pH 9	2-3
10% EtOH	< 1
95% EtOH	2-3
MeOH	3-4
$CHCl_3$	1-3
Acetone	12.5-15

Stability:

Bulk:
A sample stored at 60 °C for 10 days decomposed 18% (UV). The compound was found to be stable in bulk form at room temperature exposed to lab light through 60 days (UV, TLC and ionic chloride). For long-term storage the bulk compound should be protected from moisture and stored at -15 °C.

Solution:
The compound dissolved in 3% methanol/ water decomposed 4% in one hour, 6.5% in three hours 15% in six hours, and 38% in 24 hours (UV). There was no formation of ionic chloride during the 24 hours. Solutions should be prepared immediately before use.

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 300 x 3.9 mm i.d.
Mobile Phase:	CH_3CN/1% HOAc (aq.), 15/85, v/v
Flow Rate:	2 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.45 mg/mL in internal standard solution.
Internal Standard:	Acetonitrile containing 0.04 μL acetophenone per mL as the internal standard/1% HOAC (aq), 50/50, (v/v).
Retention Volume:	11.0 mL (NSC - 95466) 23.0 mL (I.S.)

Ultraviolet Absorption:

(3% Methanol/water)

λ_{max} = 230 ± 2nm ε = 6,052 - 6,270

Toxicity Data:

Mouse(po): LD_{50}: 35700 µg/kg
National Technical Information Service, PB282-250

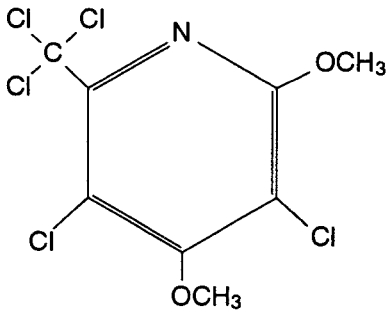
Mouse(iv): LD_{50}: 22 mg/kg
National Technical Information Service, PB282-250

Dog(iv): LD_{Lo}: 3 mg/kg
National Technical Information Service, PB282-250

Monkey(iv): LD_{Lo}: 10 mg/kg
National Technical Information Service, PB282-250

PENCLOMIDINE

NSC - 338720



Chemical Name:
3,5-Dichloro-2,4-dimethoxy-6-(trichloromethyl)pyridine

CAS Registry Number: 108030-77-9

Molecular Formula: $C_8H_6Cl_5NO_2$ **M.W.:** 325.4

Approximate Solubility:	(mg/mL)
Water	< 1
Acetate buffer (pH 4)	< 1
Carbonate buffer (pH 9)	< 1
0.1 N HCl	< 1
0.1 N NaOH	< 1
Ethanol (95%)	20-25
Methanol	30-33
n-Butanol	45-50
Acetone	> 100
Chloroform	> 100
Toluene	> 100

DMF	45-50
DMSO	45-50

Stability:

Bulk:
The bulk substance was found to be stable through 90 days when stored at room temperature and 50 °C under both light and dark conditions (HPLC).

Solution:
The compound was found to be stable in DMF/water (50/50, v/v) for at least 72 hr (HPLC).

Ultraviolet Absorption:

(methanol)

λ_{max}	ε
290 ± 2 nm	5110 ± 50
243 ± 2 nm	6990 ± 130
214 ± 2 nm	24,130 ± 1090

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 10μ, 300 x 3.9 mm i.d.
Mobile Phase:	Acetonitrile/water (65/35, v/v)
Flow Rate:	1.0 mL/min
Detection:	UV at 214 nm

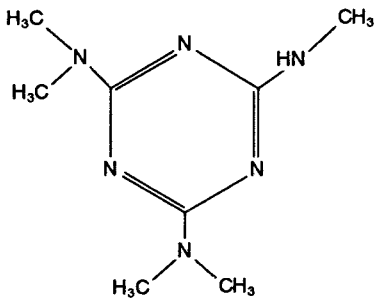
Sample Preparation: Accurately weighed samples are serially diluted wth acetonitrile to give the appropriate concentration (≈.300 to ≈1.500 mg/mL).

Internal Standard: Decanophenone, 0.3 mg/mL in mobile phase

Retention Volume: 17.3 mL (NSC 338720)
31.4 mL (I.S.)

PENTAMETHYLMELAMINE HYDROCHLORIDE

NSC - 118742



Chemical Name: *N,N,N′,N′,N″*-Pentamethylmelamine, monohydrochloride

CAS Registry Number: 35832-09-8

Molecular Formula: $C_8H_{16}N_6 \cdot HCl$ **M.W.:** 232.7

Approximate Solubility: (as free base)

Solvent	Heat	Solubility (mg/mL)
0.1 N HCl	none; moderate	≈ 15 - 20
H_2O	strong	≈ 3.6
MeOH	moderate	> 150
95% EtOH	moderate	> 200
$CHCl_3$	none	> 200
DMSO	none	> 100

Stability:

Bulk:
A sample stored at 60 °C for 30 days showed no decomposition (TLC).

Solution:
A 2% solution in water (pH = 2.9), showed no decomposition after 7 days at room temperature (TLC).

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max} = 237 ± 2 nm ε = 26,200 - 27,100

High Performance Liquid Chromatography:

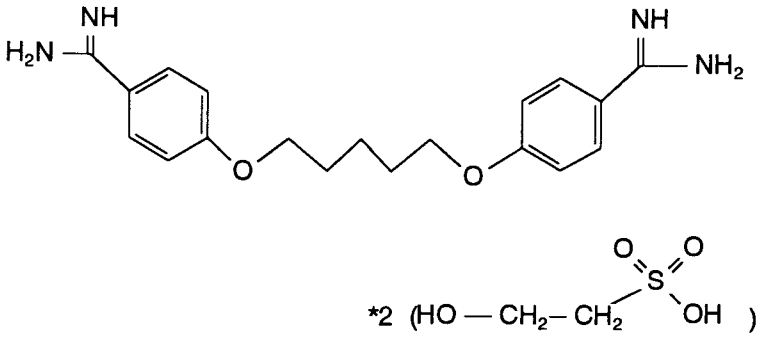
Column:	30 cm x 4.0 mm i.d. Spherisorb ODS
Mobile Phase:	MeOH/H_2O/Et_2NH, 600/400/0.5
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	1 mg samplings are accurately weighed and each dissolved in 1.00 mL H_2O. One mL of internal standard solution is added and aliquots (1.5 μL) of the resulting solutions are injected.

Internal Standard: o-nitroaniline diluted to (2.4 mg/10 mL methanol)

Retention Volume: 6.5 mL (NSC - 118742)
4.5 mL (I.S.)

PENTAMIDINE ISETHIONATE

NSC - 620107



Chemical Name: 4,4′-Diamidinodiphenoxypentane, di(β-hydroxy-ethanesulfonate)

Other Name: Pentam®300

Molecular Formula: $C_{19}H_{24}N_4O_2 \cdot 2C_2H_6O_4S$ **M.W.:** 592.8

Approximate Solubility: (mg/mL)

Water	> 30
Acetate buffer, pH 4	≈2.5
Carbonate buffer, pH 9	< 1
0.1 N HCl	≈ 2.5
0.1 NaOH	< 1
Ethanol (95%)	≈ 1.25
Methanol	≈ 1.25
Butanol	< 1
Dimethyl acetamide	≈ 15

Dimethyl sulfoxide	≈ 15
Acetonitrile	< 1
Ethyl acetate	< 1
Chloroform	< 1
Toluene	< 1

Stability:

Bulk:
The compound was found to be stable in the bulk form when exposed to light at ambient or 60 °C temperature for 90 days.

Solution:
Pentamidine isethionate was found to be stable as a solution in normal saline at room temperature over a 72 hour period.

Ultraviolet Absorption:

(methanol)

λ_{max}	ε
265± 2 nm	31400 - 80
264 ± 2 nm	30,000 - 33,000

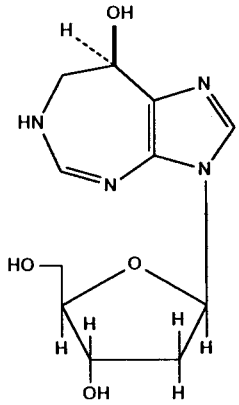
High Performance Liquid Chromatography:

Column:	Beckman Ultrasphere C_{18}, 5μ, 4.6 x 250 mm i.d.

Mobile Phase:	Acetonitrile: 2 mM Tetramethyl-ammonium Choride, pH 2.25 with phosphoric acid (45:55)
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.4 mg NSC 620107 in methanol
Internal Standard:	Butyrophenone, μL/mL in methanol
Retention Volume:	12.4 mL (NSC 620107) 19.8 mL (I.S.)

PENTOSTATIN

NSC - 218321



Chemical Name:
3-(2-Deoxy-β-*D-erythro*-pentofuranosyl)-3,6,7,8-tetrahydro-imidazo(4,5-*d*)[1,3]diazepin-8-ol, (*R*)-

Other Names: 2′-Deoxycoformycin; Co-Vidarabine

CAS Registry Number: 53910-25-1

Molecular Formula: $C_{11}H_{16}N_4O_4$ **M.W.:** 268.3

Approximate Solubility:	(mg/mL)
H_2O	> 30
pH 9 borate buffer	> 50

Stability:

Bulk:
Bulk samples stored at 60 °C for 9 days showed no decomposition (TLC and UV). Bulk material should be stored at -20 °C for long term storage.

Ultraviolet Absorption:

(pH 9 borate buffer)

λ_{max}= 283 ± 2 nm ε = 7,950 - 8,250

High Performance Liquid Chromatography:

Column:	μBondapak C_{18} 300 x 3.9 mm i.d.
Mobile Phase:	CH_3OH/0.01 M phosphate buffer (pH 7), 13/87, v/v
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.1 mg/mL in internal standard solution
Internal Standard:	acetanilide (0.3 mg/mL in mobile phase)
Retention Volume:	7.2 mL (NSC-218321) 28 mL (I.S.)

Optical Rotation:

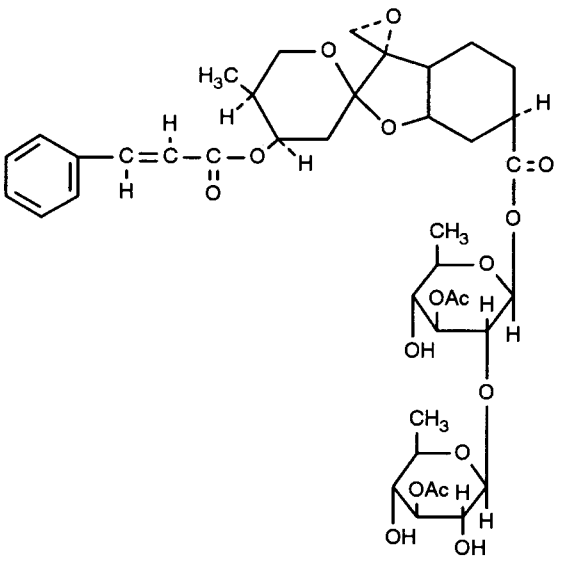
(c = 1, H_2O) $[\alpha]_D^{25} = +76.4 \pm 2°$

Toxicity Data:

Mouse(iv): LD_{50}: 122 mg/kg
National Technical Information Service, PB84-211424

PHYLLANTHOSIDE

NSC - 328426



Chemical Name:
β-*D*-Glucopyranose, 2-*O*-(3-*O*-acetyl-6-deoxy-,3-acetate 1-[decahydro-5"-methyl-4"-[1(oxo-3-phenyl-2-propenyl)-oxy]dispiro[oxirane-2,3"(2'*H*)-benzofuran-2,2"-[2*H*]pyran]-6'-carboxylate,[*2S-[2α[4R*(E),5'S*],3β,3aα,6α,7aα*]]-

CAS Registry Number: 63166-73-4

Molecular Formula: $C_{40}H_{52}O_{17}$ **M.W.:** 804.8

Approximate Solubility: (mg/mL)

H_2O	< 0.1
C_2H_5OH	> 100
$CHCl_3$	> 100
DMSO	> 100
CH_3OH	> 100
CH_2Cl_2	> 100

Stability:

Bulk:
The bulk compound is stable for at least four weeks at room temperature and 45 °C (HPLC).

Solution:
The room temperature stability in 10% aqueous ethanol (1 mg/mL) shows t_{90} to be 1.5 hours and t_{50} to be 19 hours (HPLC).

Ultraviolet Absorption:

(MeOH)

λ_{max}	ε
276 ± 2nm	20,450 - 20,730
216 ± 2nm	15,370 - 15,970
205 ± 2nm	13,820 - 14,670

High Performance Liquid Chromatography:

Column: μ-Porasil, 300 mm x 3.9 mm i.d.

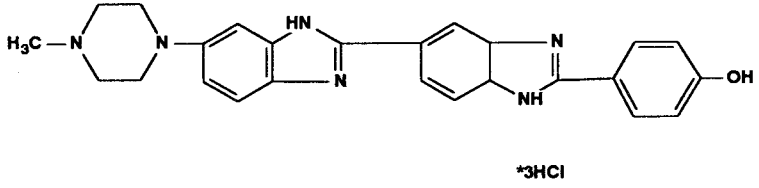
Mobile Phase:	$CH_2Cl_2/CH_3OH/H_2O$ (96/4/0.4)
Flow Rate:	0.8 mL/min
Detection:	UV at 254 nm
Sample Preparation:	One mg of sample is dissolved in 1 mL CH_2Cl_2.
Retention Volume:	11.6 mL (NSC-328426)

Optical Rotation:

(c = 0.7, $CHCl_3$) $[\alpha]_D^{20} = 17.7 \pm 2°$

PIBENZIMOL HYDROCHLORIDE

NSC - 322921



Chemical Name:

4-[5-(4-Methyl-1-piperazinyl)-[2,5′-bi-1*H*-benzimidazol]-2′-yl]-phenol, trihydrochloride

Other Names: Bisbenzimidazole

CAS Registry Number: 23491-45-4

Molecular Formula: $C_{25}H_{24}N_6O \cdot 3HCl$ **M.W.:** 534.9

Approximate Solubility:	(mg/mL)
DMSO	240 - 300
H_2O	≈ 110
95% EtOH	< 1

0.1 N NaOH	14 - 22
0.1 N HCl	43 - 44
$CHCl_3$	< 1
Acetone	< 1

Stability:

Bulk:
Under ordinary laboratory illumination, the material slowly decomposes. At the end of four weeks at room temperature in a capped glass vial, 3% decomposition has occurred (HPLC).

In a similar container but maintained at 45 °C and in darkness, the subject sample was stable for at least four weeks (HPLC).

Solution:
A solution of the sample (1 mg/mL) is stable in water for at least 24 hours at room temperature under normal laboratory illumination.

High Performance Liquid Chromatography:

Column:	Dupont Zorbax ODS, 25 cm x 4.6 mm i.d.
Mobile Phase:	0.1 M pH 7.0 KH_2PO_4/CH_3OH, 88/200
Flow Rate:	1.5 mL/min
Detection:	UV at 230 nm
Sample Preparation:	1 mg/mL in H_2O

Retention Volume: 10.95 mL (NSC-322921)

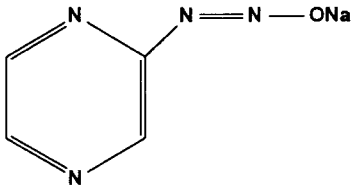
Toxicity Data:

Rat(iv): LD_{50}: 32200 μg/kg
National Technical Information Service, PB84-171206

Mouse(iv): LD_{50}: 36900 μg/kg
National Technical Information Service, PB84-171206

PYRAZINE DIAZOHYDROXIDE

NSC - 361456



Chemical Name:
N-Nitrosopyrazinamine, sodium salt

Other Names:
Sodium *N*-Nitrosopyrazinamine

CAS Registry Number: 103829-56-7

Molecular Formula: $C_4H_3N_4ONa$ **M.W.:**146.1

Approximate Solubility:	(mg/mL)
Water	> 9.3
Buffer, pH 4	> 15.2
Buffer, pH 9	> 12.8
Ethanol	7.2 - 14.4
Dimethylacetamide	> 17.4
DMSO	> 18.7
Chloroform	< 0.9
Ethyl acetate	< 0.7
t-Butanol	< 1.1

Stability:

Bulk:

The rate of degradation was variable, ranging from ≈14% at room temperature in light conditions to ≈4% under dark conditions. At 50 °C under light conditions, degradation averaged ≈4%. There was no apparent degradation at 50 °C in the dark.

Solution:

In reagent grade water, the $t_{1/2}$ was calculated to be ≈ 27.6 hr. In phosphate buffer at pH 7.32, $t_{1/2}$ was found to be 91 min. In borate buffer at pH 8.98, $t_{1/2}$ was found to be 53.8 hr.

Ultraviolet Absorption:

(methanol)

λ_{max}	ε
286 ± 5 nm	7748
254 ± 5 nm	4180

High Performance Liquid Chromatography:

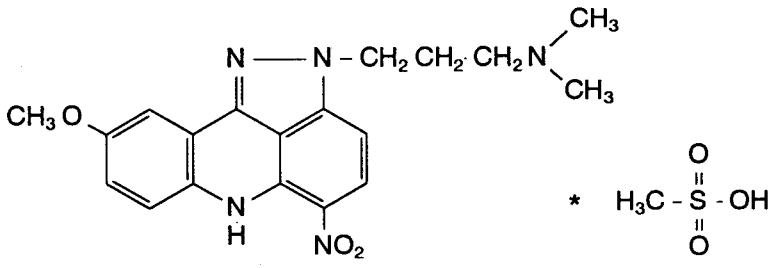
Column: PRP-1 (Hamilton Co.), 260 x 4.2 mm, with a 30 x 4.6 mm i.d. (Brownlee) guard column.

Mobile Phase: 35% Methanol/65% 0.005M phosphoric acid (0.23 mL conc. acid in 650 mL water, adjusted to pH 10 with NaOH), containing 0.005 M tetrabutylammonium hydrogen sulfate in the mobile phase.

Flow Rate:	1.5 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.5 mg/mL in Internal Standard Solution.
Internal Standard:	10mg/mL thymidine in methanol.
Retention Volume:	7.98 mL (NSC 361456) 3.05 mL (I.S.)

PYRAZOLOLOACRIDINE

NSC - 366140



Chemical Name:
9-Methoxy-*N*,*N*-dimethyl-5-nitropyrazolo[3,4,5-*kl*]acridine-2(6*H*)-propanamine, monomethanesulfonate

CAS Registry Number: 99009-20-8

Molecular Formula: $C_{20}H_{25}N_5O_6S$ **M.W.:** 463.5

Approximate Solubility:	(mg/mL)
Water	> 10.12
Buffer, pH 4	> 9.99
Buffer, pH 9	< 0.67
Ethanol	> 0.66
Dimethylacetamide	5.05 - 10.10
DMSO	> 10.18
Chloroform	< 0.68
Ethyl acetate	< 0.67
t-BuOH	< 0.67

Stability:

Bulk:
Test samples stored for 3 months at 25 °C and 50 °C under light and dark conditions showed no degradation (HPLC).

Solution:
Aqueous solutions (≈ 2 mg/mL) showed no degradation after 48 hr at 25 °C.

Ultraviolet Absorption:

λ_{max}	ε
223 ± 2 nm	39,197 - 39,537
254 ± 2 nm	11,638 - 11,878
280 ± 2 nm	8,932 - 9,004
311 ± 2 nm	12,950 - 13,000
352 ± 2 nm	6,290 - 6,415
368 ± 2 nm	7, 286 - 7,389
467 ± 2 nm	12,460 - 13,721

High Performance Liquid Chromatography:

Column:	RCM Nova-Pak
Mobile Phase:	30% CH_3CN/70% 0.1 M ammonium acetate (pH 4.4).
Flow Rate:	2.0 mL/min
Detection:	UV at 254 nm

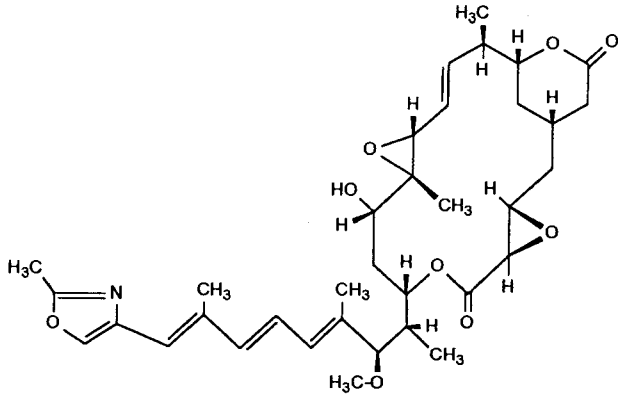
Sample Preparation: ≈ 0.4 mg/mL NSC - 366140 and 0.1 mg/mL Internal Standard in methanol.

Internal Standard: Methyl *p*-anisate

Retention Volume: 15.1 mL (NSC - 366140)
30.3 mL (I.S.)

RHIZOXIN

NSC - 332598



Chemical Name:
10-Hydroxy-8-(2-methoxy-1,3,7-trimethyl-8-(2-methyl-4-oxazolyl)-3,5,7-octatrienyl)-11,16-dimethyl-4,7,12,18-tetraoxatetracyclo(15.3.1.03,5.011,13)heneicos-14-ene-6,19-dione, (*1S-(1R*,3R*,5S*,8R*(1R*,2S*,3E,5E,7E),10R*,11S*,13S*,14E, 16S*,17S**))-

Other Names: WF 1360

CAS Registry Number: 90996-54-6

Molecular Formula: $C_{35}H_{47}NO_9$ **M.W.:** 625.8

Approximate Solubility:	(mg/mL)
H_2O	< 1
MeOH	> 50
$CHCl_3$	> 50

Stability:

Bulk:
HPLC analysis indicated that the bulk chemical is unstable under both light and dark conditions at room temperature and at 50 °C. Freezer storage is recommended.

Solution:
The compound is unstable in a solution of DMF/H_2O (40/60,v/v) through 72 hours. The t_{90} was 5.2 hours.

Ultraviolet Absorption:

(≈8 µg/mL in MeOH)

λ_{max}	ε
323 ± 2nm	39,750 ± 540
309 ± 2nm	53,260 ± 620
297 ± 2nm	42,240 ± 595

High Performance Liquid Chromatography:

Column:	Alltech Econosphere C_{18}, 5µ 250 x 4.6 mm i.d.
Mobile Phase:	CH_3CN/pH 7 phosphate buffer, 0.01 M (55/45,v/v)
Flow Rate:	1.0 mL/min
Detection:	UV at 280 nm

Sample Preparation: 11.77 mg of compound was diluted with elutent to give test sample concentrations of about 1, 0.2 and 0.02 mg/mL.

Internal Standard: Phenanthrene, 0.01 mg/mL in elutent

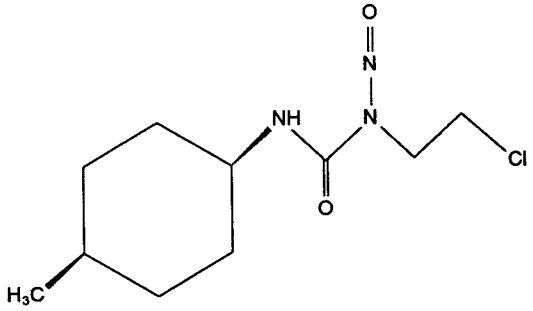
Retention Volume: 10.4 mL (NSC-332598)

Optical Rotation:

(c = 0.5, CH_3OH) $[\alpha]_D^{23} = 160 \pm 4°$

SEMUSTINE

NSC - 95441



Chemical Name:
1-(2-Chloroethyl)-3-(4-methylcyclohexyl)-1-nitrosourea

Other Name: Methyl CCNU

Molecular Formula: $C_{10}H_{18}ClN_3O_2$ **M.W. :** 247.7

Approximate Solubility:	(mg/mL)
Water	0.09
0.1 N HCl	0.09
0.1 N NaOH	0.09
10% Ethanol	0.10
Absolute Ethanol	100.00
DMSO	250.00
Chloroform	667.00

Stabilty:

Bulk:
A sample stored at room temperature for 30 days showed 4% decomposition (UV).

Solution:
A refrigerated solution in 10% EtOH decomposed 2% in 6 hours while a solution at room temperature showed 25% decomposition in 6 hours (UV). Solutions in methanol were also found to be unstable by UV analysis.

Ultraviolet Absorption:

(MeOH)

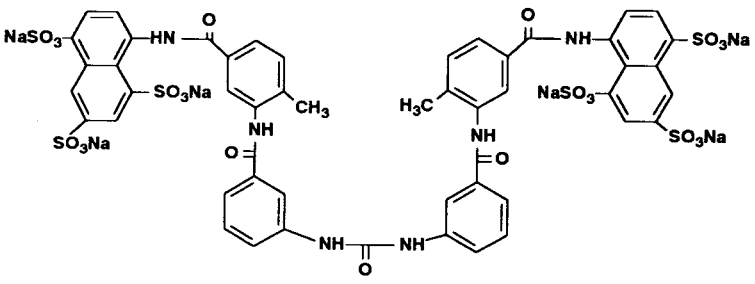
λ_{max} =229 ± 2nm ε = 6,000 - 6,190

High Performance Liquid Chromatography:

Column:	μBondpak C_{18}, 300 x 3.9 mm i.d.
Moble Phase:	CH_3CN/1% HOAc (aq), 70/30, v/v
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	Weighed amounts of the test sample (approximately 20 mg) in 10 mL flasks are dissolved in internal standard solution. These solutions are diluted 3 to 25 mL to give a concentration of 0.25 mg/mL.
Internal Standard:	Fluoranthrene (0.08 mg/mL in acetonitrile)
Retention Volume:	5.5 mL (NSC- 95441) 9.0 mL (I.S.)

SURAMIN SODIUM

NSC - 34936



Chemical Name:
8,8′-[Carbonylbis[imino-3,1-phenylenecarbonylimino(4-methyl-3,1-phenylene)carbonylimino]]bis-1,3,5-napthalenetrisulfonic acid, hexasodium salt

Other Names:
Bayer 205; 309F; Antrypol; Germanin; Moranyl; Naganol; Naganin; Naphuride Sodium

CAS Registry Number: 129-46-4

Molecular Formula: $C_{51}H_{34}N_6Na_6O_{23}S_6$ **M.W.:** 1429.2

Approximate Solubility:	(mg/mL)
Water	Very soluble
Ethyl alcohol	Slightly soluble
Chloroform	Insoluble
Ethyl ether	Insoluble

Ultraviolet Absorption:

(distilled water)

λ_{max}	ε
312 ± 2 nm	23,180 ± 70
236 ± 2 nm	108,680 ± 320

High Performance Liquid Chromatography:

Column:	μBondapak C_{18} 10μ, 300 x 3.9 mm i.d.
Mobile Phase:	Methanol/0.05 M tetrabutyl ammonium hydroxide adjusted to pH 7.4 with H_3PO_4 (65/35, (v/v)
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.05 mg/mL in methanol/0.05 M tetrabutyl ammonium hydroxide adjusted to pH 7.4 with H_3PO_4 (65/35,v/v)
Internal Standard:	Phenanthrene, 0.02 mg/mL
Retention Volume:	5.3 mL (NSC 34936) 20.1 mL (I.S.)

Toxicity Data:

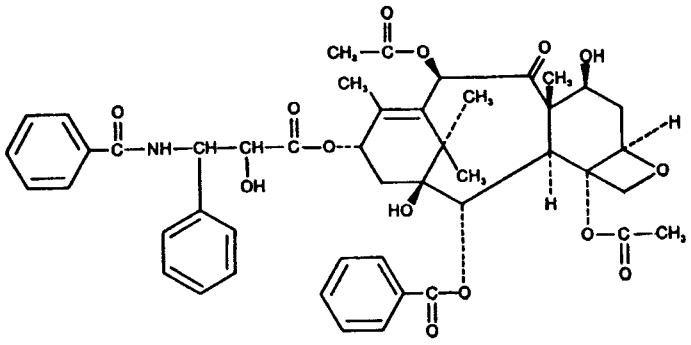
Mouse(ip): LD_{50}:750 mg/kg
Biochemical and Biophysical Research Communications,136,64,(1986)

Man(iv): TDLo:46 mg/kg/5 week intermittent schedule
New England Journal of Medicine, 314,1455,(1986)

Mouse(iv): LD_{50}:620 mg/kg
Advances in Pharmacology and Chemotherapy, 15,289,(1978)

TAXOL

NSC - 125973



Chemical Name: β-(Benzoylamino)-α-hydroxybenzenepropanoic acid, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1*H*-cyclodeca[3,4]benz[1,2-*b*]oxet-9-yl ester, [*2aR*-[*2aα,4β,4aβ,6β,9α*(α*R**,β*S**),*11α,12α,12aα,12bα*]]-

CAS Registry Number: 33069-62-4

Molecular Formula: $C_{47}H_{51}NO_{14}$ **M.W.:** 853.9

Qualitative Solubility:

Highly insoluble in water and aqueous solvents. Compound dissolves in methanol, ethanol, benzene, chloroform, methylene chloride, and tetrahydrofuran.

Stability:

Bulk:
Bulk samples stored at room temperature for 30 days showed no decomposition as indicated by UV absorption, TLC, or HPLC. The bulk compound stored at 60 °C for three weeks also showed no decomposition. After four weeks very minor decomposition was detected by TLC.

Ultraviolet Absorption:

(MeOH)

λ_{max} = 227 ± 2nm ε = 28,500 - 30,900

High Performance Liquid Chromatography:

Column:	IBM ODS, 5 μm, 4.6 x 250 mm
Mobile Phase:	63% MeOH/37% water
Flow Rate:	1.0 mL/min
Detection:	UV at 230 nm
Sample Preparation:	Dissolve ≈6 mg sample in 10 mL methanol. Mix 1 mL of this solution with 1 mL of internal standard solution.
Internal Standard:	20 mg Paraben in 25 mL methanol
Retention Volume:	19.3 mL (NSC - 125973) 7.7 mL (I.S.)

Optical Rotation:

(c = 1, MeOH) $[\alpha]_D^{20} = -53 \pm 2°$

Toxicity Data:

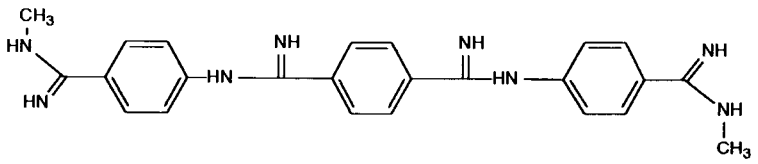
Rat(ip): LD_{50}: 32530 μg/kg
National Technical Information Service, PB83-170969

Mouse(ip): LD_{50} 128 mg/kg
National Technical Information Service, PB83-170969

Dog(iv): LD_{50}: 15 mg/kg
National Technical Information Service, PB83-170969

TEREPHTHALAMIDINE

NSC - 57155



* 4HCl

Chemical Name:

N,*N*″-Bis[4-imino-(methylamino)methyl]phenyl]-1,4-benzenedicarboximidamide, tetrahydrochloride

CAS Registry Number: 2053-23-8

Other Names: Symetamine

Molecular Formula: $C_{24}H_{26}N_8 \cdot 4HCl$ **M.W.:** 572.4

Approximate Solubility:	(mg/mL)
Water	> 10.9
Buffer, pH 4	> 10.5
Buffer, pH 9	2.1 - 2.7
Dimethylacetamide	< 0.8
Ethanol	< 0.7

DMSO	> 11.1
Chloroform	< 0.7
Ethyl acetate	< 0.7
t-BuOH	< 0.7

Stability:

Bulk:
Test samples stored for 3 months at 25 °C under light and dark conditions and at 50 °C under dark conditions showed no degradation (HPLC).

Solution:
A test sample (20 mg/mL water) exhibited no significant degradation after 48 hr at 25 °C under light (HPLC).

Ultraviolet Absorption:

(water)

λ_{max}	ε
244 ± 2 nm	27,500 - 35,900
254 ± 2 nm	26,700 - 33,750

High Performance Liquid Chromatography:

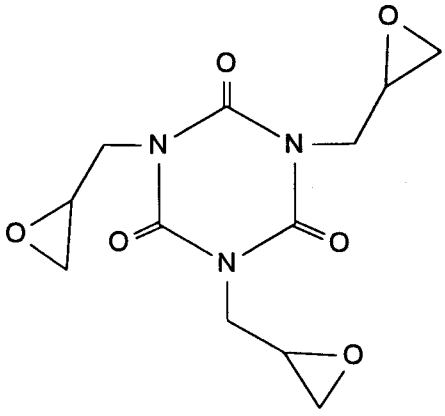
Column: Zorbax RX (C_8), 250 x 4.6 mm i.d.

Mobile Phase: 1% methanol in water containing 0.05M KH_2PO_4, pH adjusted to 3.75 with phosphoric acid.

Flow Rate:	1.5 mL/min
Detection:	UV at 254 nm
Sample Preparation:	Sample is dissolved in reagent grade water to give a concentration of ≈ 0.8 mg/mL and 0.6 mg/mL Internal Standard.
Internal Standard:	Thymine
Retention Volume:	8.0 mL (NSC 57155) 14.4 mL (I.S.)

TEROXIRONE

NSC - 296934



Chemical Name:
1,3,5-Tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione, (α)-

Other Names:
Henkel's Compound; Triazinetrione triepoxide; α-Triglycodyl isocyanurate; α-TGI

CAS Registry Number: 2451-62-9

Molecular Formula: $C_{12}H_{15}N_3O_6$ **M.W.:** 297.3

Approximate Solubility:	(mg/mL)
Water	< 1
0.1 N HCl	< 1
pH 4 buffer	2.5 - 5
pH 9 buffer	< 1
0.1 N NaOH	1 - 2.5

10% EtOH	< 1
95% EtOH	< 1

Stability:

Bulk:
After heating at 60 °C for 30 days in the dark, the sample purity dropped from > 99% to 93 ± 1%. (HPLC)

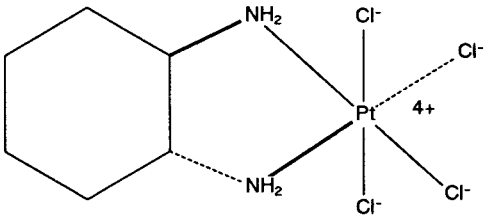
Solution:
A solution in water decomposed 29% in 72 hours. Aqueous solutions are most stable at pH 6. When acetonitrile was substituted for water as the storage solvent, < 1% decomposition was observed through 72 hours (HPLC).

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 300 x 3.9mm i.d.
Mobile Phase:	CH_3CN/H_2O, 20/80, v/v
Flow Rate:	1 mL/min
Detection:	UV at 205 nm
Sample Preparation:	1.0 mg/mL in internal standard solution
Internal Standard:	0.24 μL/mL acetophenone in CH_3CN/H_2O, 20/80,(v/v)
Retention Volume:	6.4 mL (NSC-296934) 18.5 mL (I.S.)

TETRAPLATIN

NSC - 363812



Chemical Name:
Tetrachloro(1,2-cyclohexanediamine-*N*,*N*′)platinum,[*OC*-6,22-(*trans*)]-

Other Names:
Ormaplatin (USAN); U-77-233

CAS Registry Number: 62816-98-2

Molecular Formula: $C_6H_{14}Cl_4N_2Pt$ **M.W.:** 451.1

Approximate Solubility:	(mg/mL)
H_2O	5.0 - 10.0

Stability:

Bulk:
Samples stored at 25 °C in the dark or under laboratory illumination for 90 days or at 50 °C in the dark for 90 days showed no appreciable degradation.

Solution:
The compound is unstable in aqueous solutions but is stable in normal saline for more than 24 hrs.

High Performance Liquid Chromatography:

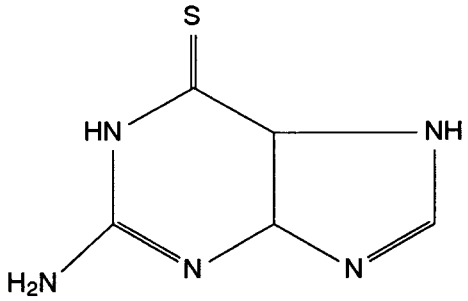
Column:	Spherisorb 5S ODS2, 250 x 4.6 mm i.d.
Mobile Phase:	2% acetonitrile in water containing 0.005 M K_2HPO_4 and 0.01 M KH_2PO_4
Flow Rate:	2 mL/min
Detection:	UV at 254 nm
Sample Preparation:	≈0.4 mg/mL in normal saline mL (I.S.)
Internal Standard:	3′-deoxyinosine (4.0 mg/mL in normal saline)
Retention Volume:	9.3 mL (NSC-363812) 17.9 mL (I.S.)

Toxicity Data:

Mouse(iv): LD_{50}: 10 mg/kg
Cancer Treatment Reports, 61,1519,(1977)

THIOGUANINE

NSC - 752



Chemical Name: 2-Amino-1,7-dihydro-6*H*-purine-6-thione

Other Names: 6-TG; 6-Thioguanine

CAS Registry Number: 154-42-7

Molecular Formula: $C_5H_5N_5S$ **M.W.:** 167.2

Approximate Solubility:

Readily soluble in dilute aqueous alkali. Insoluble in water, alcohol, or chloroform.

Stability:

Bulk:
The compound was stable in solid form at room temperature in the absence of moisture.

Solution:
Alkaline solutions slowly undergo decomposition. Alkaline solutions should not be heated above 37°C.

Ultraviolet Absorption:

(0.1N HCL)

λ_{max}	ε
257 ± 2 nm	8,000 - 8,400
347 ± 2 nm	20,600 - 30,000

High Performance Liquid Chromatography:

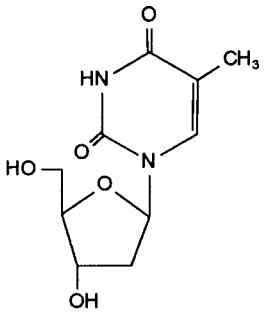
Column:	μBondapak C_{18}, 300 x 4 mm i.d.
Mobile Phase:	3% MeOH in 0.1 MKH_2PO_4, pH=4.5
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	2.0 mg/mL (0.1 N NaOH)
Internal Standard:	Thymine
Retention Volume:	10.5 mL (NSC - 752) 15.0 mL (I.S.)

Toxicity Data:

Rat (ip): LD_{50}: 300 mg/kg
Journal of Reproduction and Fertility, 4,291 (1962)

THYMIDINE

NSC - 21548



Chemical Name:
1-(2-Deoxy-β-*D*-ribofuranosyl)-5-methyl-2,4(1*H*,3*H*)-pyrimidinedione

CAS Registry Number: 50-89-5

Molecular Formula: $C_{10}H_{14}N_2O_5$ **M.W.:** 242.2

Approximate Solubility: (mg/mL)

Water	50

Stability:

Solution:
A 1% solution of thymidine in water, kept at room temperature, is stable for at least 24 hours (HPLC).

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max} = 267 ± 2 nm ε = 9,700 - 9,900

High Performance Liquid Chromatography:

Column:	Alltech Spherisorb-ODS-1, 5μ, 25 x 0.46 cm
Mobile Phase:	7% acetonitrile in 0.05M KH_2PO_4
Flow Rate:	1.0 mL/min
Detection:	UV at 255
Sample Preparation:	≈1 mg sample in 1.0 mL methanol/water or 2.0 mL internal standard solution
Internal Standard:	Adenosine (0.5 mg/mL in water)
Retention Volume:	8.5 mL (NSC - 21548) 5.9 mL (I.S.)

Optical Rotation:

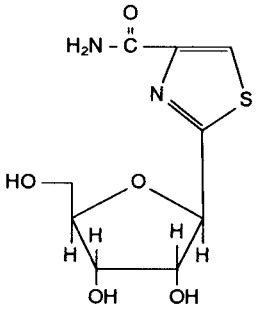
(c = 1, H_2O) $[\alpha]_D^{25}$ = +18 ± 0.5°

Toxicity Data:

Mouse(ip): LD_{50}: 2512 mg/kg
Journal of Pharmacology & Experimental Therapeutics, 207,504 (1978)

TIAZOFURIN

NSC - 286193



Chemical Name:
2-β-*D*-Ribofuranosyl-4-thiazolecarboxamide

Other Names:
TCAR; Riboxamide

CAS Registry Number: 60084-10-8

Molecular Formula: $C_9H_{12}N_2O_5S$ **M.W.:** 260.3

Approximate Solubility:

Soluble in water

Stability:

Bulk:
The compound was stable through 30 days at 60 °C in the dark (HPLC).

Solution:
In water < 1% decomposition occurs through 24 hours (HPLC).

Ultraviolet Absorption:

(95% Ethanol)

λ_{max} = 236 ± 2 nm ε = 7,660 - 7,970

High Performance Liquid Chromatography:

Column:	μBondapak C_{18}, 300 x 3.9mm i.d.
Mobile Phase:	Methanol/1% acetic acid (10/90, v/v)
Flow Rate:	1.0 mL/min
Detection:	UV at 254 nm
Sample Preparation:	0.25 mg/mL in water containing internal standard
Internal Standard:	Thymidine, 0.3 mg/mL in water
Retention Volume:	5.0 mL (NSC-286193)

Optical Rotation:

(c = 0.914, DMF) $[\alpha]_D^{25}$ = -13.8 ± 2°

Toxicity Data:

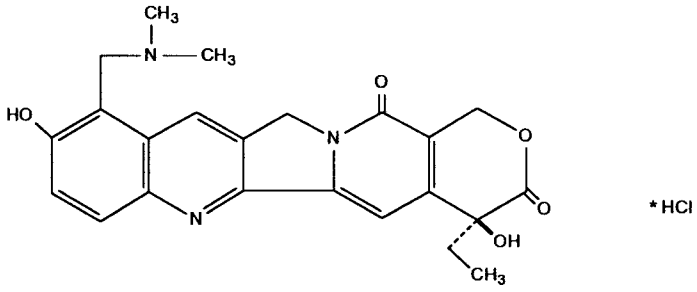
Mouse(ip): LD_{50}: 1684 mg/kg
NCI Screening Program Data Summary

Mouse(iv): LD_{50}: 3400 mg/kg
National Technical Information Service, PB83-156901

Dog(iv): LD_{Lo}: 1090 mg/kg
National Technical Information Service, PB83-156901

TOPOTECAN

NSC - 609699



Chemical Name:
4-Ethyl-4,9-dihydroxy-10-(dimethylamino)methyl]-1*H*-pyrano-[3′,4′:6,7]-indolizino[1,2-*b*]quinoline3,14(4*H*,12*H*)-dione, (*S*)-hydrochloride salt

Other Names:
SKF 104864-A; Hycamptamine

Molecular Formula: $C_{23}H_{23}N_3O_5 \cdot HCl$ **M.W.:** 457.9

Solubility:

Water	soluble
Methanol	soluble
Ethanol	insoluble
Dimethylformamide	soluble

Ultraviolet Absorption:

(MeOH)

λ_{max}	ε
207 ± 2 nm	21,484
224 ± 2 nm	39,009
269 ± 2 nm	22,902
296 ± 2 nm	6,783
318 ± 2 nm	10,003
332 ± 2 nm	13,091
371 ± 2 nm	19,267
384 ± 2 nm	22,718

High Performance Liquid Chromatography:

Column: Zorbax RX, 250 x 4.6 mm i.d. (Waters Assoc.), with a universal prefilter (Alltech)

Mobile Phase: 15% CH_3CN/0.1M ammonium acetate, adjusted to pH 4.0 with acetic acid.

Flow Rate: 1.2 mL/min

Detection: UV at 254 nm

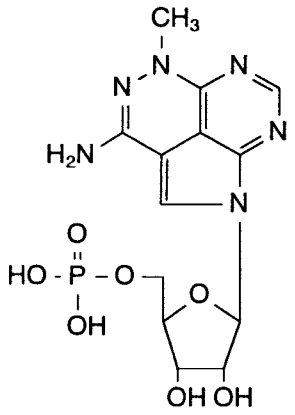
Sample Preparation: Sample is dissolved in methanol to provide a solution having ≈0.45 mg/mL of Topotecan and 0.22 mg/mL Internal Standard.

Internal Standard: p-Hydroxyacetophenone

Retention Volume: 13.4 mL (NSC - 609699)
16.0 mL (I.S)

TRICIRABINE PHOSPHATE

NSC - 280594



Chemical Name:
1,5-Dihydro-5-methyl-1-(5-*O*-phosphono-β-*D*-ribofuranosyl)-1,4,5,6,8-pentaazaacenaphthylen-3-amine, monohydrate

Other Names:
Tricyclic Nucleoside 5′-Phosphate

CAS Registry Number: 61966-08-3

Molecular Formula: $C_{13}H_{17}N_6O_7P \cdot H_2O$ **M.W.:** 418.3

Approximate Solubility: (mg/mL)

MeOH	< 1
DMSO	1 - 5
DMF	< 1
Trifluoroacetic acid	> 50
H_2O	< 1

pH 4 Acetate buffer	< 1
pH 9 Borate buffer	1 - 5
pH 9 Carbonate buffer	10 - 15
0.1 N HCl	< 1
10% EtOH	< 1
95% EtOH	< 1

Stability:

Bulk:
A sample stored at 60 °C for 30 days showed no decomposition (TLC or UV).

Solution:
A solution (.0156 mg/mL) in pH 9 carbonate-bicarbonate buffer showed no decomposition after 9 days (UV).

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{max} = 292 ± 2 nm ε = 11,700 - 12,500

High Performance Liquid Chromatography:

Column:	μBondapak C_{18} 300mm x 3.9 mm i.d.
Mobile Phase:	Methanol/pH 7 0.01 M phosphate buffer with 0.005 M tetrabutyl-ammonium hydroxide 25/75, v/v.
Flow Rate:	1 mL/min

Detection: UV at 254 nm

Sample Preparation: pH 9 carbonate buffer containing internal standard

Internal Standard: acetanilide

Retention Volume: 25.6 mL (NSC-280594)

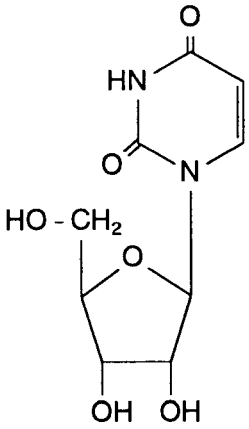
Toxicity Data:

Mouse(ip): LD_{50}: 193 mg/kg
NCI Screening Program Data Summary

Mouse(iv): LD_{50}: 109 mg/kg
NCI Screening Program Data Summary

URIDINE

NSC - 20256



Chemical Name:
1-β-*D*-ribofuranosyluracil

CAS Registry Number: 58-96-8

Molecular Formula: $C_9H_{12}N_2O_6$ **M.W.:** 244.2

Qualitative Solubility:

Soluble in H_2O, and DMSO. Insoluble in ether and hexane

Ultraviolet Absorption:

(pH 7 buffer)

λ_{max} = 261 ± 2 nm ε = 9,600 - 10,200

High Performance Liquid Chromatography:

Column:	4.6 mm x 25 cm ODS Spherisorb 10
Mobile Phase:	0.5 M pH 6.6 KH_2PO_4 buffer/CH_3OH, 19/1
Flow Rate:	1.5 mL/min
Detection:	UV at 254 nm
Sample Preparation:	1.3 mg/mL in mobile phase
Internal Standard:	1 mg adenosine/2mL water
Retention Volume:	5.7 mL (NSC - 20256)

Optical Rotation:

(c = 2, H_2O) $[\alpha]_D^{20} = 9.4 \pm 2°$

Toxicity Data:

Mouse(ip): LD_{50}: 4335 mg/kg
Journal of Pharmacology & Experimental Therapeutics, 207,504,(1978)

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